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National Aeronautics and
Space Administration

George C. Marshall Space Flight Center
Marshall Space Flight Center, Alabama 35812

**THE LEWIS CHEMICAL EQUILIBRIUM PROGRAM
WITH PARAMETRIC STUDY CAPABILITY**

MAY, 1981



Prepared for:

NASA/George C. Marshall Space Flight Center
Huntsville Computer Complex

(NASA-CR-161811) THE LEWIS CHEMICAL
EQUILIBRIUM PROGRAM WITH PARAMETRIC STUDY
CAPABILITY (Computer Sciences Corp.) 287 P
HC A13/MF A01 CSCL 21D

NE1-26275

Unclas
63/28 26739

Prepared by:

Computer Sciences Corporation
Engineering Systems Department
Project Development and Systems Support Section

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(Organization(s) that prepared this report:)

COMPUTER SCIENCES CORPORATION

THE LEWIS CHEMICAL EQUILIBRIUM PROGRAM
WITH PARAMETRIC STUDY CAPABILITY

MAY, 1981

Prepared by:

Pere' levigny
Senior Computer Scientist

Reviewed by:

David B. Johnson, Manager
Project Development and Systems Support Section

Robert H. Johnson, Manager
Engineering Systems Department

ABSTRACT

The program is a modification of the Lewis Chemical Equilibrium program to extend the usefulness of the program in a Coal Gasification Study. A previous version adapted the original program to allow direct input of coal composition data. The current revision adds a capability for parametric studies of various coal gasification factors. In addition, an optional data file collection system was implemented for use with the parametric studies. The program was also converted to operate under ASCII FORTRAN rather than FORTRAN V on the UNIVAC 1100/82.

The program works on single precision data in an interactive mode and uses approximately 32k of core. There are no special input/output requirements beyond a single system tape.

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1.0 INTRODUCTION

1.1 OBJECTIVE

The Coal Gasification Task Team required parametric studies of several factors involved in the coal gasification process. The parametric studies involve the combination of parameters such as oxygen/coal and water/coal ratios over ranges of the individual parameters.

This program was developed to automate the process of running all of the possible combinations of the factors under study. The factors to be varied are entered as a list of values to be computed and the program automatically sets all of the necessary combinations of variables and runs the complete gasification calculation for each combination.

The problem which is solved by the program is the addition of a parametric case study capability to the existing Lewis Chemical Equilibrium Program. Various parametric data are entered by the user and printed data are created covering the possible combinations of the original data.

This program was developed for the Computer Services Office (AH33) in support of activities in the Coal Gasification Task Team (PF15) under contract NAS8-31640.

1.2 MSFC FORM 3559

(See the following page.)

REQUEST FOR COMPUTER SERVICES SUPPORT
USER RESOURCES PROJECTION PLAN
HUNTSVILLE COMPUTER COMPLEX

1. NAME OF REQUESTER (24 characters): Jon French		4. NAME OF PROJECT (36 characters): TVA Coal Gasification	
2. TELEPHONE NUMBER: 453-4024	3. ORGANIZATION (14 characters): PA01	PROJECT (UNIVAC 1100) 778-44-29	5. DATE OF REQUEST 8/8/80

JOB NUMBER	SERIES CODE	COG. ACT.	PROJECT	SYSTEM
	-	P A	- 7 7 8 -	R 5 0 0 7 1

6. JOB TITLE (24 characters):
TVA Coal Gasification

7. JOB DESCRIPTION (300 characters):
Provide flow sheet graphics; absorption, stripping, and distillation column design; facility and equipment sizing and plant layout; startup procedure timelines; and analyses of: cost and economics, material and energy balance, combustion equilibrium for the TVA Coal Gasification facility.

19 81 FISCAL YEAR RESOURCES PLAN

ESTIMATED HOURS/SUP						COST
	1ST. QTR	2ND. QTR	3RD. QTR	4TH. QTR	TOTAL	
LABOR	10. 1926	11. 1927	12. 1926	13. 1927	14. 7706	15. \$105,957.50
COMPUTER	16. 10	17. 11	18. 10	19. 11	20. 42	21. \$5,880.00
23. COMPUTER IDENTIFICATION: UNIVAC 1100						22. TOTAL COST: \$111,837.50

8. FUNDING SOURCE: ☐ R&PM ☐ D&O ☐ R&D ☒ REIMBURSABLE

9. WORK PACKAGE: **34X** 26. TASK NUMBER: 27. TASK TITLE (24 characters):

10. NAME OF PROGRAMMER/ANALYST (24 characters): Mike Fague	29. NAME OF MANAGER (24 characters): Mike Fague	30. ORGANIZATION: 653
11. NAME OF MONITOR (24 characters): R. Marden	32. TELEPHONE NUMBER: 3-2294	33. ORGANIZATION: 71133

12. COMMENTS:
Scientific/Engineering

ORIGINAL PAGE IS
OF POOR QUALITY

34

<input type="checkbox"/> OVERSIGHTS	36. SIGNATURE OF AUTHORIZED REQUESTER: Ries H. Ince	37. DATE RECEIVED:
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1.3 BACKGROUND

The original Lewis Chemical Equilibrium Program (Reference 1) was developed to determine chemical equilibrium in complex systems. Using a free-energy minimization technique, the program permits calculations such as:

- Chemical Equilibrium for assigned thermodynamic states (T,P), (H,P), (S,P), (T,V), (U,V), OR (S,V),
- Theoretical rocket performance for both equilibrium and frozen compositions during expansion,
- Incident and reflected shock properties,
- Chapman-Jouget detonation properties. The program considers condensed species as well as gaseous species.

It has been shown (Reference 2) that the same program can handle solid coal in an entrained flow coal gasification problem. Since the original program was not designed for coal input, the calculations necessary to change the coal data into the proper form are long and tedious. The automation of the calculation process is documented in Reference 2.

The problem of parametric studies in the original program is complicated, because the original program made no provision to vary the factors of interest in coal gasification studies. The current program was created to reduce the need for user intervention at every step of the parametric studies.

2.0 PROGRAM TASK DESCRIPTION

The Lewis Chemical Equilibrium Program was revised to include the following capabilities:

1. Accept a data set which can be used to create a series of runs covering the variations of one parameter as other independent variables are changed. All of the variables which are being changed affect the coal composition. Previous versions of the program had to restate the coal composition between each calculation. The current process does all of the calculations automatically once the calculation values have been entered.
2. Create, as a user option, a data file which contains a condensation of the data calculated in the multiple runs. The option can also be used to collect single data points or any combination.
3. Run under ASCII FORTRAN rather than FORTRAN V.

A complete listing of the source code, after alterations, is given in Appendix A. A complete listing of the original, pre-alteration, coding is included as Appendix B, so that the differences can be traced.

3.0 METHOD OF SOLUTION

The solution of the problem, as described in the Task Description, involved creating storage area to hold the parametric data and the plot output data. In addition, logic had to be added to force the system to loop through the parametric values in a planned fashion and to store the plot data as required. The conversion to ASCII FORTRAN from FORTRAN V also introduced revisions, principally in the area of character manipulation and core overlay.

A detailed description of the effect that the task solution had on each subroutine is given in the following pages.

3.1 STORAGE ELEMENT A (Map Overlay Source Code)

The subroutine COALCV was divided into a driver (COLCV) and 3 subroutines (COLCV1, COLCV2, COLCV3); the subroutine OUT1 was divided into 4 subroutines (OUT1, OUT2, OUT3, OUT4). The subroutine SAVE was divided into 2 subroutines (SAVE, NEWOF). The overlay structure was revised to reduce the core requirement, since the ASCII level generated larger elements. The split in COALCV also ties in with the use of multiple runs, see COLCV3.

3.2 STORAGE ELEMENT BLOCK 1 (Miscellaneous data - Block Data Form)

The Hollerith data was revised to match ASCII requirements. In particular, the contents of COMMON area OUTP were extensively revised.

3.3 STORAGE ELEMENT BOOT (Bootstrap Control Section)

No changes

3.4 STORAGE ELEMENT CHECK (Subroutine Check)

No changes. Note CHECK is not actually used in the program but was included because it is on the system tape.

3.5 STORAGE ELEMENT COALCV (Subroutine COALCV)

The original COALCV was replaced with a driver for COLCV1, COLCV2 and COLCV3. The 3 subroutines, together, are equivalent to the old COALCV. The split was arranged partly to produce smaller segments but, primarily to enable subroutine COLCV3 to be entered independently of the other two.

3.6 STORAGE ELEMENT COLCV1 (Subroutine COLCV3)

The subroutine contains the portion of old subroutine COALCV which reads in and displays old coal data, as required,. It also determines whether the existing coal data is to be completely replaced or modified. The particular sections to be modified are also identified.

3.7 STORAGE ELEMENT COLCV2 (Subroutine COLCV2)

The subroutine contains the portion of old subroutine, COALCV, which reads in the required coal data. This may be an entire set of new data or selected replacements of existing data. New functions are put in to rearrange the oxidizer list, so that oxygen is always first. The "other fuel" section is rearranged so that water is first. Also the variable recycle carbon to coal ratio is computed. This value is stored as an additional entry in COMMON and CFUEL. It also applies to COALCV, COLCV1 and COLCV3.

3.8 STORAGE ELEMENT COLCV3 (Subroutine COLCV3)

The subroutine contains the portion of the old subroutine COALCV which does the calculations to convert raw coal composition data into reactant data acceptable to the equilibrium calculation program. In addition, the subroutine serves the purpose of introducing 3 parameters which are part of the possible variations of the multiple runs.

The three parameters are percent carbon conversion, water to coal ratio, and recycle carbon to coal ratio. The parameters enter the subroutine as arguments in the call list. If the value of the argument is negative, then the existing value of the

argument, as taken from the coal data file, is used in the calculations. If the argument is positive, then the call argument is used in place of the original argument in all of the composition calculations. The subroutine COLCV3 is called separately from COLCV1 and COLCV2 when changes in the coal composition data are required by changes to the three parameters. (See subroutine MAIN.)

The other addition to COLCV3 is the storage of certain computed data into a storage area of the COMMON block DPLOT. Storage occurs only if a plot flag has been set in subroutine MAIN. Table 1 indicates the meaning of the various storage values. Not all of the storage slots are filled by COLCV3. Other slots are filled by various other subroutines as the data becomes available.

TABLE 1**PLOT DATA VALUES**

<u>VARIABLE NUMBER</u>	<u>MEANING</u>
1	Oxygen/Coal Ratio
2	Steam/Coal Ratio
3	Carbon Conversion Function
4	Recycle Carbon/Coal Ratio
5	Fuel/Coal Ratio
6	Weight Fraction C in Coal
7	Weight Fraction H in Coal
8	Weight Fraction N in Coal
9	Weight Fraction O in Coal
10	Weight Fraction S in Coal
11	Weight Fraction as in Coal
12	Coal Temperature °F
13	Higher heating value of Coal Btu/lb
14	Steam Temperature °F
15	Weight Fraction Oxygen in Oxidizer
16	Oxidizer Temperature °F
17	Pressure PSIA
18	
19	Future Expansion
20	
21	Mixture Molecular Weight
22	Mixture Temperature °F
23	Mixture Enthalpy Btu/Lb

24	Mixture Mole Fraction of CO
25	Mixture Mole Fraction of CO ₂
26	Mixture Mole Fraction of CH ₄
27	Mixture Mole Fraction of H ₂
28	Mixture Mole Fraction of H ₂ S
29	Mixture Mole Fraction of COS
30	Mixture Mole Fraction of N ₂
31	Mixture Mole Fraction of AR
32	Mixture Mole Fraction of H ₂ O
33	Mixture Mole Fraction of C(S)
34	Mixture Mole Fraction of IC(S)
35	Mixture Mole Fraction of HCL
36	Mixture Mole Fraction of HCN
37	Mixture Mole Fraction of NH ₃
38	Mixture Mole Fraction of S
39	Mixture Mole Fraction of (solids & liquids)
40	
41	
42	
43	Future Expansion
44	
45	

3.9 STORAGE ELEMENT CPHS (Subroutine CPHS)

Rearrangement of COMMON area SPECES to allow for more useable equivalence statements in other subroutines. Increased array A from 15 x 150 to 25 x 150 to allow for an expansion from 15 to 25 reactants. This last change was missed in the previous revision.

3.10 STORAGE ELEMENT DETON (Subroutine DETON)

Changed COMMON area OUPT as indicated in BLOCK1. Also changed Hollerith data to fit into the ASCII character format.

3.11 STORAGE ELEMENT EQLBRM (Subroutine EQLBRM)

Changed COMMON area SPECES as indicated in Section 3.9.

3.12 STORAGE ELEMENT FROZEN (Subroutine FROZEN)

Changed COMMON area SPECES as indicated in Section 3.9.

3.13 STORAGE ELEMENT GAMEFF (Subroutine GAMEFF)

No changes.

3.14 STORAGE ELEMENT GAUSS (Subroutine GAUSS)

No changes

3.15 STORAGE ELEMENT GETON (Partial control stream)

The group of control statements labeled GETON is used, via ADD, to reinitialize the system after having terminated control.

3.16 STORAGE ELEMENT HCALC (Subroutine HCALC)

Changed common area SPECES as indicated in Section 3.9.

3.17 STORAGE ELEMENT LTCPHS (Subroutine LTCPHS)

No changes.

3.18 STORAGE ELEMENT MAIN (System Driver)

Changes in COMMON area SPECES as indicated in Section 3.9. Addition of variable CCR to COMMON area CFUEL. Addition of COMMON area DSAVE to provide storage which will not be destroyed when subroutine THERMP is overlaid. Addition of COMMON area DPLOT to provide temporary storage for plot data.

To hold the parameters needed for the multiple runs, the namelist CDATA was added. Table 2 shows the components of the namelist. Note that for each combination of OXCOAL, PCTCNV, RCCOAL, up to six variations of WCOAL may be used. In addition to the 60 possible combinations which can be used to calculate equilibrium compositions, a secondary quench composition can be calculated by setting QT to TRUE and assigning values to IQTYPE and TA. A total of 120 runs can be created with one set of data with no further operator intervention.

In the initialization section, file 11 is opened via a DEFINE FILE. The file is used to accumulate the plot data as one record per combination of variables. Also, the material in the CDATA list is initialized.

Immediately after the section which reads in the namelist INPT2, a new section is added which does exactly the same thing for CDATA. The user is given the choice of using the existing data and replacing pieces of it, or initializing the entire group and reading in entirely new data. The new CDATA material is stored on file 10 after the INPT2 data.

When execution is actually started, option 7, the user is given a choice as to whether or not to print the CDATA material. The INPT2 data is always printed. At this point the user is asked whether or not plot data storage is required. An answer of "yes" requests a code name (16 characters) to associate with the data group, sets the plot counter to 1 and then asks whether a tape already exists. If such a tape exists, then the user should already have copied it into file 11. The first record on the file gives the number of records on the file and the record number of the next record to fill.

TABLE 2

COAL DATA NAMELIST (CDATA)

OXCOAL (10)	Oxygen to coal ratio
PCTCNV (10)	Percent carbon conversion
RCCOAL (10)	Recycle carbon to coal ratio
WCOAL (5,10)	Water to coal ratio: (Each combination of oxygen to coal, percent conversion and recycle carbon to coal may have up to 6 water to coal ratios.)
QT	True or False, Indicates whether a quench temperature calculation is to be performed.
IQTYPE	Integer which specifies process 1 KOPPERS-TOTZEK 2 TEXACO
TA	Quench temperature for Texaco

The program then computes the number of oxygen to coal compositions and the number of sets of water to coal compositions. If both are zero, the program will run without any use of the multiple run option.

The temporary parameters of percent conversion, recycle carbon to coal and water to coal ratio are set. Note that the maximum number of water to coal values is calculated for the combination of other variables. The data from INPT2 is obtained from file 10 and the MIX value is set to the oxygen to coal ratio. When quench calculations are required during the second pass (IQT=1); then selected values of the INPT2 variable are set depending on which process is being calculated. For the first pass (IQT=0), subroutine COLCV3 is called to work the new parameters into the coal composition data. The processing then continues in the normal function, except that after subroutine REACT, the special omits and the inert carbon insertions are omitted any time the REPEAT flag is on.

Processing is normal until after the call to subroutine THERMP. At this point, the REPEAT flag is set on if any of the flags indicating multiple runs are on. Then the programming returns to run other cases. The order is Quench calculations, additional water to coal ratios and then oxygen to coal ratios.

When all of the multiple run cases for the set of data have been completed, normal processing resumes. Before returning to the menu for new input, the stored plot data record on file 11 is closed, if the plot flag is on. The number of records associated with the given data is added to the first record of the particular set. The first record on the file is updated to point to the next available record.

3.19 STORAGE ELEMENT MATRIX (Subroutine MATRIX)

Changed COMMON area SPECES as indicated in Section 3.9.

3.20 STORAGE ELEMENT NEWOF (Subroutine NEWOF)

The subroutine consists of the entry NEWOF of the old subroutine SAVE. Note that there was no overlap between the SAVE and NEWOF entries. The only other change was the addition of variable CCR to COMMON area CFUEL.

3.21 STORAGE ELEMENT OUT1 (Subroutine OUT1)

The subroutine consists of the entry OUT1 of the old subroutine OUT1. The old subroutine consists of four entries, OUT1, OUT2, OUT3 and OUT4 which were all independent of each other. The entire were split into independent subroutines to reduce core requirements in the overlay.

Other changes were the addition of variable CCR to COMMON area CFUEL, the addition of COMMON area DPLOT and the rearrangement of some Hollerith data to fit the ASCII requirements. Also, some of the plot data is stored. Note that each plot variable has 13 storage slots.

During the ordinary multiple run cases, usually only one condition is used at a time. The other slots are allocated for use when the program is run with multiple pressures or temperatures.

3.22 STORAGE ELEMENT OUT2 (Subroutine OUT2)

The subroutine consists of the entry OUT2 of the old subroutine OUT1 (see Section 3.20). Other changes were the addition of variable CCR to COMMON area CFUEL, the addition of COMMON area DPLOT and the revision of COMMON area OUPT, as indicated in Section 3.2. Various parts of the plot data are also stored in the subroutine.

3.23 STORAGE ELEMENT OUT3 (Subroutine OUT3)

The subroutine consists of the entry OUT3 of the old subroutine OUT1 (see Section 3.20). The extra changes are the addition of variable CCR to the COMMON area CFUEL and the revision of COMMON area OUPT as in Section 3.2 and the revision of COMMON area SPECES as in Section 3.9. No plot data is saved in this section.

3.24 STORAGE ELEMENT OUT4 (Subroutine OUT4)

The subroutine consists of the entry OUT 4 of the old subroutine OUT1 (see Section 3.20). Changes in the data areas include the addition of variable CCR to COMMON area CFUEL, the revision of COMMON area SPECES as in Section 3.9 and the addition of COMMON area DPLOT. Hollerith data indicating the species which are to be stored in the plot area were also added.

In addition to the original calculations, the mole fractions of the various designated species are stored in the plot area. The mole fractions of any solids and liquids which are not in the designated list are summed and stored in the plot area.

3.25 STORAGE ELEMENT PLOTBOOT (Partial Control Stream)

The set of control statements is used, via ADD, to set the plot data file for additions to the file. The + in statement 3 is replaced with the actual number of the tape on which the plot data is being accumulated.

3.26 STORAGE ELEMENT PLOTSAVE (Partial Control Stream)

The control statements are used to transfer the accumulated print data from the mass storage file to tape. The tape is the same as that from which the data originated. The overwrite feature is to be used.

3.27 STORAGE ELEMENT PROK (PDP Element PROK)

Changed COMMON area SPECES as indicated in Section 3.9.

3.28 STORAGE ELEMENT REACT (Subroutine REACT)

The changes in the data areas included the addition of variable CCR to COMMON area CFUEL, and the addition of COMMON area QUENCH and DSAVE. QUENCH contains the material needed to compute the quench calculations. DSAVE stores material which must be preserved against being overlaid.

The only addition to the logic of the subroutine involves the quench enthalpy calculation. Quench calculations pass through subroutine REACT twice. On the first pass, IQT is 0 and normal calculations are done. If QT is true, IQT is reset to 1 and the next pass will do the quench calculations.

The type of calculations depends entirely on the process being investigated. For the Koppers-Totzek process, the enthalpy for each component of the normal calculation is adjusted by

$$H_q = H_a - 9.75 \times 10^{-12} T_a^4 \text{ (MW)}$$

Where:

H_q is the quench enthalpy (cal/g)

H_a is the mixture enthalpy calculated for a normal run (cal/g)

T_a is adiabatic flame temperature corresponding to H_a ($^{\circ}\text{K}$)

MW molecular weight of the component

For the Texaco process, the calculation is done by running the entire computation at constant T_a rather than at the constant pressure of the original runs.

Note that in either case, when $\text{IQT}=1$, the existing reactant data is reused rather than starting from the reactant file data. The only difference is that the existing data has all of the enthalpies, either calculated or given, while the reactant file has only the given enthalpies. For both cases, the asterisk which indicates that a given enthalpy should be calculated is suppressed in the reactant listing. For the Koppers-Totzek case, the enthalpy calculation flag is reset to zero to force a recalculation for every component.

3.29 STORAGE ELEMENT RKTOUT (Subroutine RKTOUT)

Changed COMMON area SPECES as discussed in Section 3.9. Changed COMMON area OUPT as discussed in Section 3.2.

3.30 STORAGE ELEMENT ROCKET (Subroutine ROCKET)

No changes

3.31 STORAGE ELEMENT RREAD (Subroutine RREAD)

The Hollerith data used to form headers and titles was reworked to conform to ASCII conventions.

3.32 STORAGE ELEMENT SAVE (Subroutine SAVE)

The subroutine is the portion of the old subroutine SAVE which corresponds to the entry print SAVE. (See NEWOF, Section 3.19).

3.33 STORAGE ELEMENT SEARCH (Subroutine SEARCH)

Changed COMMON area SPECES as discussed in Section 3.9.

3.34 STORAGE ELEMENT SHCK (Subroutine SHCK)

Changed COMMON area SPECES as discussed in Section 3.9. Changed COMMON area OUPY as discussed in Section 3.2.

3.35 STORAGE ELEMENT TAPESAVE (Partial Control Stream)

Added statement 8 to get tape numbers of saved tape automatically.

3.36 STORAGE ELEMENT THERMP (Subroutine THERMP)

Changed COMMON area OUPY as discussed in Section 3.2. COMMON area DPLOT was added.

After the call to OUT4, the stored plot data from DPLOT is moved to file 11 if the plot flag is on and the record counter is incremented by the number of records added.

3.37 STORAGE ELEMENT VARFMT (Subroutine VARFMT)

Common area OUPF was changed as discussed in Section 3.2.

3.38 THERMODYNAMIC DATA (FILE 4)

No changes.

In addition to the previously discussed changes, all of the subroutines were reworked to conform to ASCII level 9 FORTRAN conventions. Principally, this applied to character data.

4.0 PROGRAM DESCRIPTION

The program is run in interactive mode on the UNIVAC 1100/82 machine under the EXEC 8 operating system. The program is written in ASCII FORTRAN and requires only the normal FORTRAN library routines.

The program operates in approximately 32K and uses a single input system tape.

5.0 OPERATING INSTRUCTIONS

Table 3 shows a typical set of data for a multiple run. The total number of runs to compute this data would be 36×2 . There are 36 water/coal combinations and the quench calculation doubles the number of runs.

The problem involving gasification of Kentucky #9 coal in a Texaco process using an oxidizer stream of almost pure oxygen and with a recycle stream (other fuels) as indicated in Table 3. The system pressure is 15 psia and the temperatures of the various streams are as indicated. The primary parametric factors under consideration are the oxygen to coal ratio and the water to coal ratio. Carbon conversion and recycle carbon to coal ratio are dependent on the oxygen to coal ratio for this particular coal gasification process.

The following pages trace the steps involved in setting up the program and show a typical set of output data.

Note that an answer of 'YES' to the question "PRINT TO PRINT FILE" would place most of the output onto a previously defined alternate file (31).

For option 8, entering the coal data, the particular data already existed on the tape. For examples of how to enter a completely new set of data or to edit existing data, see "Addition to the Lewis Chemical Equilibrium Program to Allow Computation from Coal Composition Data". (Reference 2.)

For option 6, entering namelist variable, the namelist CDATA shows the setup to compute all of the requirements of Table 3 in one pass.

TABLE 3
TEXACO WITH RECYCLE

COAL, KY#9, T=200°F, P=15 psia

carbon conversion - see table

other fuels - all @ T=200°F lb/lb coal

Al₂O₃ .07466

SiO₂ .1983

FeO, .08678

Water (l), See table

Recycle carbon, See table

Oxidizer T=221°F

.975 O₂

.025 AR

Slag \ ash	.70	.65	.63	.60	.55	.50
------------	-----	-----	-----	-----	-----	-----

OXYGEN COAL	CARBN CONV.	RECYCLE		WATER/COAL				
		CARBON/ COAL	CARBON/ COAL					
.85	.9137	.0606	.5087	.7648	.8342	.9469	1.1621	
.90	.9429	.0379	.5990	.7526	.8209	.9318	1.1436	1.3977
.95	.9622	.0236	.5929	.7449	.8125	.9223	1.1319	1.3834
1.00	.9750	.0145	.5890	.7400	.8071	.9152	1.1244	1.3743
1.05	.9834	.0085	.5865	.7368	.8037	.9123	1.1196	1.3684
1.10	.9890	.0047	.5848	.7347	.8014	.9097	1.1164	1.3645

Quench Calculations Required - Quench Temperature 2000°F

For option 7, startup, the listing of CDATA shows only the one test case which matches the output data.

Note that an answer of 'YES' to the 'SAVE PLOT DATA' will produce a request for a code name of 16 characters to associate with the data. It will also produce a question as to whether the plot tape is blank or already contains other plot data.

The first set of output is the normal calculation. The second set is for the quench calculation. Note that the special omit data section only occurs for the first data set.

Note that on exiting, if the alternate print file has been designated, then the user is required to take the appropriate steps to cause the alternate print file to be printed.

5.1 TEST CASE

See following pages.

```

20ESTPM: USERID/PASSWORD ENTRY
P M L 1100 OPERATING SYSTEM LEV. C0302280071(001)S
P M L DAY 5-18-81 FROM 15:48 TO 18:00 ESTESTESTEST ESTESTESTESTEST
P M L LEVIST 11M001050021 SEVU0001N000.30.000
DATE 051881 TIME 150430
>?T
OFFEE TPF8
READY
>0ASG. T TPF8.F/3/005/3
READY
>0ASG. T PLR.U95.13202
READY
>0COP...G PLR .TPF8
FURPUR 28R1M1 E36 574711 05/18/81 15:05:30
SEVU0001N000LEU15(1) COPIED ON 05/14/81 AT 18:30 48
132 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
>0ADD TPF8 BOOT
READY
READY
READY
READY
READY
READY
READY
READY
READY
READY
FURPUR 28R1M1 E36 574711 05/18/81 15:09:31
132 BLOCKS COPIED
SEVU0001N000LEU15(1) COPIED ON 05/14/81 AT 18:31:10
17 BLOCKS COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVU0001N000LEU15(1) COPIED ON 05/14/81 AT 18:31:19
1 BLOCK COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVU0001N000LEU15(1) COPIED ON 05/14/81 AT 18:31:23
1 BLOCK COPIED
EOF ENCOUNTERED ON INPUT TAPE
SEVU0001N000LEU15(1) COPIED ON 05/14/81 AT 18:31:26
1 BLOCK COPIED
EOF ENCOUNTERED ON INPUT TAPE
READY
>0XOT LEU1 B
READY
>0XOT
>0XOT LEU15 B

```

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- 0 - TERMINATE PROGRAM
- 1 - INSERT THERMODYNAMIC DATA
- 2 - INSERT LOW TEMP EXTENSION THERMO DATA
- 3 - INSERT OR EDIT REACTANTS
- 4 - OMIT SPECIES FROM THERMO DATA
- 5 - INSERT CONDENSED SPECIES
- 6 - INSERT OR EDIT NAMELIST
- 7 - START PROGRAM CALCULATION
- 8 - INSERT OR EDIT COAL DATA

>5

TYPE YES TO READ IN PREVIOUS COMPOSITION

>YES
1 - VOLATILE (OPTIONAL) AND (ASH AS LBS/100 LBS DRY COAL
VOLATILE 37 5400
ASH 15 8300

2 - COAL TEMPERATURE IN DEG F 200 00

3 - DR/ COAL COMPOSITION AS LBS/100 LBS DRY COAL

C 67 3100
H 4 7570
N 1 5200
O 6 3430
S 4 1000

4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, STATE AND COMPONENT
1310 G CL 2 0000 0000 0000

5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT

53 6800
26 0200
20 2300

SI 1 0000 0
FE 2 0000 0
AL 2 0000 0

6 - FRACTION CARBON CONVERSION 9137

7 - HEATING VALUE OF COAL IN BTU/LB 12141 000

8 - OTHER FUEL COMPONENT AS LBS/LB COAL, TEMPERATURE IN DEG F, STATE AND COMPONENT

6887 200 000 L H 2 0000 0 1 0000
0747 200 000 S AL 2 0000 0 2 0000
1983 200 000 S SI 1 0000 0 2 0000
0863 200 000 S FE 1 0000 0 1 0000
0606 200 000 S C 1 0000

9 - OXIDIZER TEMPERATURE IN DEG F 221 00

10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND COMPONENT

97 5000
2 5000

O 2 0000
AR 1 0000

TYPE 1 TO MODIFY, 2 TO REPLACE OR 0 TO CONTINUE
>0

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- 0 - TERMINATE PROGRAM
- 1 - INSERT THERMODYNAMIC DATA
- 2 - INSERT LOW TEMP EXTENSION THERMO DATA
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- 5 - INSERT CONDENSED SPECIES
- 6 - INSERT OR EDIT NAMELIST
- 7 - START PROGRAM CALCULATION
- 8 - INSERT OR EDIT COAL DATA

>6

TYPE YES FOR PRINT INPT8 NAMELIST
>
BEGIN NAMELIST INPT8 INPUT
> INPT8 MP. T. P-18 SEND

TYPE VES FOR PRINT OF C-DATA NAMELIST

```

> BEGIN NAMELIST C-DATA INPUT
> A-DATA ODCOML 85 20 95 1 00 1 05 1 10
> B-TIME 3137 3429 3622 3750 3834 3890
> C-COML 0006 0379 0436 0146 0086 0047
> D-COML 1 11 0087 7648 3342 9469 1 1821
> E-COML 1 21 0000 7526 8209 9318 1 1436 1 13077
> F-COML 1 31 0000 7449 8125 9223 1 1319 1 3834
> G-COML 1 41 0000 7449 8071 9162 1 1244 1 3743
> H-COML 1 51 5855 7368 8037 9123 1 1106 1 3684
> I-COML 1 61 5845 7347 8014 9097 1 1164 1 3645
> J- : : IGTYP=2 TA *2000 SEND

```

PAUSE 00000 >

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LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- 0 - TERMINATE PROGRAM
 - 1 - INSERT THERMODYNAMIC DATA
 - 2 - INSERT LOW TEMP EXTENSION THERMO DATA
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 - 4 - OMIT SPECIES FROM THERMO DATA
 - 5 - INSERT CONDENSED SPECIES
 - 6 - INSERT OR EDIT NAMELIST
 - 7 - START PROGRAM CALCULATION
 - 8 - INSERT OR EDIT COAL DATA
- >>

TYPE YES FOR PRINT TO ALTERNATE PRINT FILE

TYPE YES FOR PRINT TO ALTERNATE PRINT FILE

> SINGP2
DETH - F.ERATIO - F.FA - F.FPCT - F.HP - T.IDEBUG - 0.10ms - F.
MIX - 00000000 00000000 00000000 00000000 00000000 00000000
P - 15000000+002 00000000 00000000 00000000 00000000 00000000
T - 00000000 00000000 00000000 00000000 00000000 00000000
U - 00000000 00000000 00000000 00000000 00000000 00000000
SEND

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1

5-13

TIME YES TO SAVE PLOT DATA

PAUSE 00000)

1998

POLICE 00000 >

	ALCL3	ALCL3	ALCL3(S)		FE(S)	FECL3(S)	FECL3	FLORENZ	HWCO	NE	Cl(S)	NO3	NO3S	SO	SiO2
J 6/78										J 3/61					
J 12/83										J 6/65					
J 6/78										J 6/65					
J 12/83										J 12/84					
J 3/81										J 12/84					
J 12/78										J 12/85					
J 9/85										J 6/71					
J 3/87										J 9/67					
J 3/61										J 9/67					
J 6/81										J 9/67					
J 3/65										J 9/67					
J 12/78										J 9/67					
J 6/85										J 9/67					
J 12/86										J 9/67					
J 3/85										J 9/67					
J 12/78										J 9/67					

OF - 419000 OXIDIZER/COAL- 8500 WATER/COAL- 8887 CARBON CONVERSION- 9137 RECYCLE CARBON/COAL- 8886

FUEL OXIDANT MIXTURE

M. CAL G - 19993638+004 17813499+002 - 140281E4+004

KG-ATOMS/KG

C 27512511-001 00000000 19388550-001

H 56575136-001 00000000 39869492-001

N 53810044-003 00000000 37920884-003

O 25781406-001 60939785-001 36163957-001

S 63031531-003 00000000 44419427-003

IC 25986532-002 00000000 18313165-002

CL 18214694-004 00000000 12836215-004

SI 23241327-002 00000000 16378571-002

FE 84702655-003 00000000 59691449-003

AL 10319858-002 00000000 78785922-003

AR 90000000 62581365-003 18479174-003

PT C H N O S IC CL SI FE AL AR

1 - 799 -9 248 -14 890 -41 291 -16 155 -1 337 -40 841 -2 848 13 262 -9 139 -24 943 24 000

1 -1 400 -9 225 -14 974 -39 857 -16 184 -1 401 -39 292 -3 780 12 149 -55 870 -25 974 7 000

1 -1 731 -9 222 -15 007 -39 838 -16 186 -1 428 -34 769 -4 199 -4 964 -54 685 -25 124 8 000

1 -6 998 -9 656 -15 447 -30 516 -15 043 -1 931 -31 874 -33 273 -5 145 -39 822 -25 714 9 000

1 -6 977 -9 654 -15 446 -30 548 -15 045 -1 929 -31 884 -33 267 -5 142 -39 875 -25 711 2 000

1 -9 482 -10 519 -15 140 -32 606 -12 961 -1 579 -32 520 -48 627 -9 533 -54 189 -25 303 6 000

1 -6 982 -9 656 -15 442 -30 561 -15 038 -1 906 -31 891 -33 461 -5 524 -39 376 -25 708 9 000

PAUSE 000000 >

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED PRESSURES

CHEMICAL FORMULA										UT FRACTION										ENTHALPY										STATE										TEMP										DENSITY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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OXIDIZER/COAL- 8600 WATER/COAL- 8887 CARBON CONVERSION- 9137 RECYCLE CARBON/COAL- 8888

MOLE FRACTIONS

AL2O3(S)	8 238-883
AR	4 187-883
CH4	4 688-886
CO	3 389-881
COS	3 681-884
CO2	1 888-881
FeO(S)	1 382-888
H	5 148-887
HCL	2 987-884
H2	8 822-881
H2O	1 596-881
H2S	9 674-883
IC(S)	4 148-882
NH3	1 414-886
N2	4 295-883
SH	5 752-886
S2	7 436-886
SiO2(S)	3 711-882
HHU COAL B/LB	12141 88
MIXTURE RU	22 658
MF OF CDG	72867
V SAT SCF/LB	35 78811
HHU SAT B/SCF	266 83
EFFICIENCY	78479
V DRY SCF/LB	35 17972
HHU DRY B/SCF	278 84
LHU SAT B/SCF	247 68
LHU DRY B/SCF	251 48
B PER MBTU	2 48

PAUSE 88888 >

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED QUENCH TEMPERATURE

CHEMICAL FORMULA										UT FRACTION		ENTHALPY		STATE	TEMP DEG K	DENSITY G/CM3
												CAL/MOL				

OXIDIZER/COAL- 8640 WATER/COAL- 8487 CARBON CONVERSION- 8137 RECYCLE CARBON/COAL- 8888

MOLE FRACTIONS

ALB03(S)	8 229-003
AR	4 187-003
CH4	1 486-006
CO	3 277-001
CO2	3 878-004
CO2	1 818-001
FE01(S)	1 352-002
FE02H2	6 189-007
H	1 487-006
HCL	2 908-004
HE	2 753-001
H2O	1 684-001
H2S	9 825-003
IC(S)	4 149-002
NA3	1 842-006
NE	4 295-003
SH	1 311-005
SO2	1 100-005
S2	1 844-005
SI02(S)	3 711-002
MMU COAL B/LB	12141 00
MIXTURE MW	22 658
MF OF CDC	72288
V SAT SCF/LB	35 37636
MMU SAT B/SCF	289 32
EFFICIENCY	78474
V DRY SCF/LB	34 85288
MMU DRY B/SCF	273 36
MMU SAT B/SCF	259 45
MMU DRY B/SCF	254 21
B PER MMBTU	2 49

PAUSE 00000 >

LEWIS CHEMICAL EQUILIBRIUM PROGRAM

MAIN MENU

- 0 - TERMINATE PROGRAM
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- 2 - INSERT LOW TEMP EXTENSION THERMO DATA
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- 6 - INSERT OR EDIT NAMELIST
- 7 - START PROGRAM CALCULATION
- 8 - INSERT OR EDIT CORL DATA

OF IN

RUNID LEVIST ACCT IMPADISE0021 PROJECT SEVIONBND00
LOAD 1252 TP14 PUB -1 LEVIST
SERVICE TP14 13052 LEVIST
LEVIST ABORT
LEVIST ABORT FIN
TIME TOTAL 00 01 27 248 CBSLPS 017201152
CPU 00 00 18 083 I/O 00 00 47 918
CC/ER 00 00 26 348 WAIT 00 29 12 388
IMAGES READ 100 PAGES 13
START 15 04 30 MAY 18.1081 FIN 15 39 13 MAY 18.1081

INITIAL USE OF LABELED FR80 TAPES HAS IDENTIFIED A PROBLEM #####
PLEASE DISCONTINUE USE OF LABELED FR80 TAPES UNTIL FURTHER NOTICE

STERMINAL INACTIVES
>

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6.0 REFERENCES

1. "Computer Program for Calculations of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shock and Chapman - Jouget Detonation" Gordon and McBride, NASA SP-273, 1971.
2. "Addition to the Lewis Chemical Equilibrium Program to Allow Computation from Coal Composition Data", Sevigny NASA Marshall Space Flight Center, 1981.

APPENDIX A

SOURCE LISTING OF PROGRAM ELEMENTS WITH MODIFICATIONS

This is a printout of the Lewis Chemical Equilibrium Program with the modifications required for the multiple runs.

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SEVIGNA1M2080TPF,101,A

1 LIB LEWIS.
2 LIB SYSGRAPHICS.
3 LIB SYSTEMSFC.
4 NOT FTMPTOT,FTMPH02,FTMPH03,FTMPH04,FTMPH05
5 SEG DRIVE.
6 IN LEWIS,LOCK1
7 IN LEWIS,MAIN
8 SEG 000,(DRIVER)
9 IN LEWIS,COALCV
10 SEG 0010,(100)
11 IN LEWIS,COLCV1
12 SEG 0020,(100)
13 IN LEWIS,COLCV2
14 SEG 0030,(100)
15 IF LEWIS,COLCV3
16 SEG 010,(DRIVER)
17 IN LEWIS,AREAD
18 SEG 020,(DRIVER)
19 IN LEWIS,REACT
20 SEG 030,(DRIVER)
21 IN LEWIS,LTCPHS
22 SEG 040,(DRIVER)
23 IN LEWIS,SEARCH
24 SEG 0510,(DRIVER)
25 IN LEWIS,VARENT
26 SEG 051A,(051)
27 IN LEWIS,OUT1
28 SEG 051B,(051)
29 IN LEWIS,OUT2
30 SEG 051C,(051)
31 IN LEWIS,OUT3
32 SEG 05100,'051)
33 IN LEWIS,OUT4
34 SEG 0520,(DRIVER)
35 IN LEWIS,HCALC
36 IN LEWIS,CPMS
37 SEG 05200,(052)
38 IN LEWIS,SAVE
39 SEG 05200,(052)
40 IN LEWIS,NEWOF
41 SEG 060,1051A,051B,051C,051D,052A,052B)
42 IN LEWIS,EQLBRM
43 IN LEWIS,MATOTX
44 IN LEWIS,GAUSS
45 SEG 070,(106)
46 IN LEWIS,THERMP
47 SEG 080,(106)
48 IN LEWIS,DEION
49 SEG 090,(106)
50 IN LEWIS,SMCK
51 SEG 100,(106)
52 IN LEWIS,ROCKET
53 IN LEWIS,PKTOUT
54 IN LEWIS,EROZEN
55 IN LEWIS,GAMEFF

AMDS-P BLOCK1

DATE 051403

BLOCK 1

56. X FOUR/SHF9.9./,FP/6MPC/P (ONE/SHF9.1/ZERO/SHF9.0./
57. .VCE/SHF9.1./,FG/76MKS VE/TSV76MKSIN VE/

58. X THREE/SHF9.3./,TWO/SHF9.2./

59. DATA FG11/'GAMMA ' /FG12/'COS' //

60. DATA FI11/'ISP SE' /FI12/'COMOS' //

61. DATA FI11/'IVAC S' /FI12/'SECONDS' //

62. DATA FI11/'MOL ' /FI12/'WEIGHT' //

63. DATA FI11/'MACH N' /FI12/'NUMBER' //

64. DATA FI11/'IDLV/D' /FI12/'LEP' T' //

65. DATA FI11/'IDLV/D' /FI12/'LTP' P' //

66. DATA FI11/'PRESS' /FI12/'M/M002' //

67. DATA FI11/'CP CAL' /FI12/'IGOK' //

68. DATA FI11/'STAR' /FI12/'MSEC' //

69. DATA FI11/'ENTH C' /FI12/'AL/G' //

70. DATA FI11/'S CAL' /FI12/'TBT' T' //

71. DATA FI11/'TEMP D' /FI12/'EG. N' //

72. DATA FI11/'L M/SE' /FI12/'C' //

73. DATA END/3MEND/GAS/IMS/IE/IMS/IZERO/2MOO/LANK/2M /,MOL/LHM/

74. 1 .OK/IMO/ZERO/IMO/.ATHN/101325.0/.RVR/P2.0550977/

75. 3 .LGMET/9.8006650/.PATM/19.6960050/.RPAR/1.9871650/.ROR/0.319.290360/

76. END

. 1YH00060

END FTH 1062 COMMON

3M06,P B00T

3PRT,S B00T

FURPUR 2AR1M1 E36 574T11 05/14/81 16:30:51

100

SEVIGWBIM200778707-0007
2CAT.61207-0007
FBI/DOJ
FBI/DOJ

1	6WBTW20	ACAT, P 12, F 10/10	12P
2	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
3	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
4	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
5	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
6	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
7	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
8	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
9	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
10	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
11	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
12	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
13	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
14	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
15	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P
16	ACAT, P 12, F 10/10	ACAT, P 12, F 10/10	12P

AMDG, P
CHECK

CHECK

REFIN.S CHECK.CHECK

FTN 9012005/10/81-1613010,1

SUBROUTINE CHECKNAME1

2. C
3. C
4. DATA IOLNM,2M /,IMIGH/IMZ/,ILOW/IMA/
DATA UNION=0,LOW=0,ICHAR1=0,ICHAR2=0

5. BITS(ICHAR1,31,61)=BITS(NAME,1,61)
6. BITS(ICHAR2,31,61)=BITS(NAME,1,61)
7. BITS(IMIGH,31,61)=BITS(IMIGH,1,61)
8. BITS(LOW,31,61)=BITS(LOW,1,61)
9. IF(ICHAR1.LI.JLOW.OR.ICHAR1.GT.JHIGH) NAME=IOLNM2
10. IF(ICHAR2.LI.JLOW.OR.ICHAR2.GT.JHIGH) NAME=IOLNM2

11. IF(ICHAR2.LI.JLOW.OR.ICHAR2.GT.JHIGH)
12. X BITS(NAME,7,61)=BITS(IOLNM,7,61)
13. RETURN
14. END

END FTN 95 IOLNM 10 IOLNM

AM06.P CONTIN

COALCV

DATE 051081

PAGE 1

BTWPS COALCVCOALCV

FTW 0912005/14/81-16:10(31)

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1. SUBROUTINE COALCV(FIRST)
2. C USE MIPS INPUT ROUTINES TO READ COAL CONVERSION
3. C END CREATE SIMULATED PERCENTAGE CARDS
4. COMMON FUEL/CF,MHV,MCR,PER,CCR
5. COMMON /CCCVCOALCV,JOPT,DEMAND
6. LOGICAL FIRST
7. C ARRAYS FOR COAL DATA
8. CHARACTER*4 ICAL,ICCOMP,IOFUEL,IOXID,IACOMP
9. C DIMENSION PROH(3),ICAL(14),ICOMP(15),CCOMP(16),VIECOMP(16,5),
10. C OXID(17,10),IOFUEL(16,10),OXID(16,5),IOXID(15,5),
11. C ACOMP(16,10),IACOMP(15,10)
12. DIMENSION MH(18)
13. COMMON /COALCV/PROH,ICAL,ICCOMP,IOFUEL,IOXID,IACOMP,OFUEL,OXID,
14. C CIEMP,OTEMP,IE,MH,MCOAL,MASH,MFUEL,NOXID
15. COMMON /CMHDATA/ICOMP,IACOMP,IOFUEL,IOXID
16. DIMENSION JOPT(110)
17. CALL MEMPHS
18. NREAC=0
19. IOPT=0
20. DO 2 I=1,10
21. Z JOPT(I)=1
22. CALL COALCV1(FIRST,JOPT,IOPT)
23. IF IOPT.EQ.01 RETURN
24. CALL COALCV2(JOPT,IOPT)
25. IF I.EQ.1
26. IMCH=1
27. CALL COALCV3(TPER,TCCR,TCCR)
28. RETURN
29. END

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END FTW 06 1600 42 00000 359 COMMON

ENDG.P COALCV

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1. SUBROUTINE COLCVT(FIRST,JOPT,IOP1)
2.   USE MIPS INPUT ROUTINES TO READ COAL CONVERSION
3.   AND CREATE SIMULATED REAGENT CARDS
4.   COMMON /CFUEL/CF,MHVV,MCRPER,CCR
5.   COMMON /CCOAL/COAL,ICOMP,TOFUEL,TOXID,I'COMP
6.   LOGICAL FIRST
7.   ARRAYS FOR COAL DATA
8.   CHARACTER*8 I'COAL,ICOMP,TOFUEL,TOXID,I'COMP
9.   DIMENSION PROX(1),COAL(5),ICOAL(5),ACOMP(6,5),
10.    OFUEL(7,10),TOFUEL(6,10),OXID(6,5),IOXID(5,5),
11.    ACOMP(6,8),I'ACOMP(6,8)
12.   DIMENSION MHBI
13.   COMMON /COMMON/PROX,COAL,ICOMP,ACOMP,OFUEL,OXID
14.   C TEMPT,TEMP,IE,MH,MCOAL,NASH,MFUEL,M'CHD
15.   COMMON /COMMON/YICVAL,ICOMP,INCOMP,TOFUEL,TOXID
16.   DIMENSION JOPT(10)
17.   CHARACTER*4 TOIST
18.   CHARACTER*4 YFS,YVES
19.   DATA I(1),I(1,5),I'(1,5),M',M',O',S'/
20.   DATA IC/12/
21.   DATA YVES/'YES '/
22.   IOPT=-1
23.   DO 12 I=1,5
24.     12 ICOAL(I)=IO(I)
25.     C FOR FIRST PASS DO NOT CHECK SAVED DATA
26.     IF (.NOT.FIRST) GO TO 10
27.     WRITE ('(60F10.000)')
28.     10000 FORMAT('I TYPE YES TO READ IN PREVIOUS COMPOSITION')
29.     READ ('(10000)') YES
30.     IF (YES.ME.YVES) GO TO 300
31.     10 CONTINUE
32.   C READ IN PREVIOUS COAL DATA
33.   REMIND IC
34.   READ ('C') MOUNTY,CEN,MHVV,MCR,PER
35.   READ ('C') PROX,(ICOAL(I),COAL(I),I=1,5),PER,IE,MH
36.   READ ('C') MCOAL,NASH,MFUEL,NOXID
37.   READ ('C') (ICOMP(I),J,ICOMP(I,J),I=1,6),J=1,MCOAL,
38.    I'ACOMP(I),I'ACOMP(I,J),I=1,5),J=1,MASHT,
39.    I'OFUEL(I),I'OFUEL(I,J),I=1,5),J=1,MFUCLT,
40.    I'OXID(I),I'OXID(I,J),I=1,5),J=1,MORXD)
41.   C DISPLAY PRESENT COAL DATA
42.   IF (FIRST) GO TO 50
43.   WRITE ('(OUT,10000)')
44.   READ ('5,10000') YES
45.   IF (YES.ME.YVES) GO TO 50
46.   50 CONTINUE
47.   WRITE ('(OUT,10010)')
48.   10010 FORMAT('1 - VOLATILE (OPTIONAL) AND ASM AS LBS/100 LBS ')
49.   X 'OPY COAL'
50.   WRITE ('(OUT,10012)') PROX(1),PROX(3)
51.   10012 FORMAT('X,VOLATILE',F10.4,'/6X,ASM',5x,F10.4)
52.   WRITE ('(OUT,10020)') TEMPT

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56. 10020 FORMAT 1, 2, 3 - COAL TEMPERATURE IN DEG F, F10.2, 1, 2
57. X 3 - DRY COAL COMPOSITION AS LBS/100 LPS DRY COAL
58. DO 66 121, 5
59. WRITE (JOUT, 62) ICOAL(1), COAL(1)
60. 62 FORMAT (5X, 10X, 10X, 10X, 10X, 10X)
61. 66 CONTINUE
62. WRITE (JOUT, 10030)
63. 10030 FORMAT 1, 2, 3, 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY
64. X 4 - COAL STATE AND COMPONENT
65. IF INCOAL.EQ.0 GO TO 80
66. DO 72 121, 4COAL
67. WRITE (JOUT, 70) CCOMP(1, 1), ICCOMP(1, 1),
68. X 1 - CCOMP(1, 1), ICCOMP(1, 1), J=2, 4
69. 70 FORMAT (F10.4, 10X, 4, 512X, A2, 2X, F8.4)
70. 72 CONTINUE
71. 80 WRITE (JOUT, 10040)
72. 10040 FORMAT 1, 2, 3, 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND
73. X 5 - COMPONENT
74. IF INASH.EQ.0 GO TO 90
75. DO 88 121, 5ASH
76. WRITE (JOUT, 84) ACOMP(1, 1),
77. X 1 - ACOMP(1, 1), ACOMP(1, 1), J=1, 5
78. 84 FORMAT (F10.4, 10X, 5, 12X, A2, 2X, F8.4)
79. 88 CONTINUE
80. 90 WRITE (JOUT, 10050) PER
81. 10050 FORMAT 1, 2, 6 - FRACTION CARBON CONVERSION, F10.4)
82. WRITE (JOUT, 10060) WHIE(1)
83. 10060 FORMAT 1, 2, 7 - HEATING VALUE OF COAL IN BTU/LB, F13.3)
84. 10070 WRITE (JOUT, 10070) OTHER FUEL COMPONENT AS LBS/100 COAL,
85. X 7 - TEMPERATURE IN DEG F, STATE AND COMPONENT
86. IF IMPUCEL.EQ.0 GO TO 104
87. DO 102 121, NFUEL
88. WRITE (JOUT, 10080) OFUEL(1, 1), OFUEL(2, 1), OFUEL(3, 1),
89. X 1 - OFUEL(1, 1), OFUEL(2, 1), OFUEL(3, 1), J=1, 5
90. 10080 FORMAT (F10.4, F10.3, 1X, A3, 512X, A2, 2X, F8.4)
91. 102 CONTINUE
92. 104 WRITE (JOUT, 10090) TEMP
93. 10090 FORMAT 1, 2, 9 - OXIDIZER TEMPERATURE IN DEG F, F10.2)
94. WRITE (JOUT, 10090)
95. 10090 FORMAT 1, 2, 10 - OXIDIZER COMPONENTS AS LBS/100 LBS
96. X 10 - OXIDIZER AND COMPONENT
97. IF INOXID.EQ.0 GO TO 112
98. DO 110 121, NOXID
99. WRITE (JOUT, 100) OXID(1, 1), OXID(2, 1), OXID(3, 1), J=1, 5
100. 100 FORMAT (F10.4, 10X, 512X, A2, 2X, F8.4)
101. 110 CONTINUE
102. 112 WRITE (JOUT, 10100)
103. 10100 FORMAT 1, 2, 11 - TIME 1 TO MODIFY 3 TO REPLACE OR 0 TO CONTINUE
104. 10100 FORMAT 1, 2, 11 - TIME 1 TO MODIFY 3 TO REPLACE OR 0 TO CONTINUE
105. 10100
106. 114 CONTINUE
107. READ (5, *) IOPT
108. IF IOPT.LT.0 OR IOPT.GT.2 GO TO 114
109. IF IOPT.EQ.0 RETURN
110. GO TO 120, 1001, 1002
111. C SELECT GROUPS TO BE CHANGED
112. 120 CONTINUE

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A-13

ORIGINAL PAGE IS
OF POOR QUALITY

COLCV1

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113. DO 129 1-1,10
114. 129 JOPT11=0
115. WRITE (JOPT1,102001)
116. 10200 FORMAT (' TYPE GROUP NUMBERS OF DATA TO BE CHANGED ',
117. ' IN ASCENDING ORDER. FOR EXAMPLE, 1 3 7 97')
118. 126 CONTINUE
119. READ (5,91) (JOPT11),J=1,10)
120. DO 130 1-10,1,-1
121. JJ=JOPT11)
122. IF (JJ.EQ.0) GO TO 130
123. JOPT11)=0
124. JOPT11)=JJ
125. 130 CONTINUE
126. C ADD OR UPDATE COAL DATA
127. 300 CONTINUE
128. RETURN
129. END

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END FTM 224 IBANK 836 DRANK 369 COMMON

END,P COLCV2

A-16

COLV2

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111. 10050 FORMAT 1, TYPE LINE NUMBER, 1)
112. 2300 L=0
113. READ (5,0) LM
114. IF (LM,LE,0,0,LM,GT,0,0) GO TO 2300
115. IF (INOUT,EO,1) GO TO 2366
116. C
117. DELETE
118. L=L+1
119. IF (LM,EO,0,0,LM,GT,0,0) GO TO 2366
120. DO 2362 L=L+1,NASH
121. DO 2361 J=1,5
122. ACOMP(J,1)=ACOMP(J,1)
123. 2361 IACOMP(J,1)=IACOMP(J,1)
124. 2362 ACOMP(J,1)=IACOMP(J,1)
125. 2363 NASH=NASH+1
126. GO TO 2352
127. C
128. ALTER
129. 2364 N=L+1
130. GO TO 2372
131. C
132. ADQ
133. 2370 NASH=NASH+1
134. N=NASH
135. READ IN NEW DATA
136. 2372 WRITE (JOUT,10050)
137. 10050 FORMAT 1, LOS/100 LOS DRY ASH AND COMPONENTS
138. 00 2370 J=1,5
139. IACOMP(J,1)=N
140. 2370 ACOMP(J,1)=IACOMP(J,1)
141. 2371 IACOMP(J,1)=IACOMP(J,1)
142. 2372 IACOMP(J,1)=IACOMP(J,1)
143. GO TO 2352
144. C
145. 2380 FES2=0.
146. 00 2380 J=1,5
147. 00 2380 J=1,5
148. IF (IACOMP(J,1),NE,IACOMP(J,1)) GO TO 2384
149. IF (IACOMP(J,1),NE,IACOMP(J,1)) GO TO 2384
150. 2384 CONTINUE
151. FES2=ACOMP(1,1)
152. GO TO 300
153. 2386 CONTINUE
154. GO TO 300
155. 351 COMT.NUE
156. C
157. 10050 FORMAT 1, TYPE LOS/100 LOS DRY ASH FOR COMPONENTS
158. 10050 FORMAT 1, TYPE LOS/100 LOS DRY ASH FOR COMPONENTS
159. X STATE ASSUMED SOLID; COMT. TEMPERATURE ASSUMED.
160. WRITE (JOUT,10060)
161. 10060 FORMAT 1, 302
162. READ (5,0) ACOMP(1,1)
163. WRITE (JOUT,10061)
164. 10062 FORMAT 1, FES2
165. READ (5,0) ACOMP(1,1)
166. WRITE (JOUT,10063)
167. 10063 FORMAT 1, AL2O3
168. READ (5,0) ACOMP(1,1)
169. WRITE (JOUT,10064)

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COLC42

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170. 100000 FORMAT (1, F52.1)
171.  READ (5,0) ACOMP(1,1)
172.  J=0
173.  C  REMOVE ANY ZERO COMPONENTS
174.  DO 366 J=1,6
175.  IF (ACOMP(1,1)) .366.
176.  CONTINUE
177.  ACOMP(1,1)=ACOMP(1,1)
178.  IF (11-NE-J) ACOMP(1,1)=0
179.  DO 362 LL=1,5
180.  ACOMP(LL,1)=A25M(1,LL)
181.  362 ACOMP(LL,1,1)=ASH(1,LL,1)
182.  366 CONTINUE
183.  NI=J+1
184.  C  ADD OTHER ASH COMPONENTS
185.  WRITE (JOUT,10070)
186.  10070 FORMAT (1, CONTINUE WITH ASH COMPONENTS)
187.  IF (105/100 L65 DRY ASH AND COMPONENT)
188.  CONTINUE
189.  367 DO 368 J=1,5
190.  ACOMP(J,1,1)=0
191.  368 ACOMP(J,1,1)=2
192.  ACOMP(1,1)=0
193.  READ (5,0) ACOMP(1,1), (1,1) ACOMP(J,1,1), ACOMP(J,1,1), J=1,5)
194.  IF (ACOMP(1,1)) 370, 372, 370
195.  370 NI=NI+1
196.  372 JC=367
197.  375 NI=NI+1
198.  CONTINUE
199.  C  PERFORM CONVERSION FUNCTION
200.  WRITE (JOUT,10080)
201.  10080 FORMAT (1, TYPE CONVERSION FUNCTION FUNCTION FOR ELEMENT 0-000)
202.  READ (5,0) PER
203.  C  COMPUTE VALUES FOR MW BY DIFFERENT FORMULAS
204.  390 CONTINUE
205.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
206.  X  .90*50*COAL(4)
207.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
208.  X  .90*50*COAL(4)
209.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
210.  X  .55*50*COAL(5)
211.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
212.  X  .55*50*COAL(5)
213.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
214.  X  .55*50*COAL(5)
215.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
216.  MW(1)=105.00*COAL(1)+620.20*COAL(2)+0.125*COAL(3)
217.  DO 392 J=1,6
218.  ENCODE (390,0,0,0) MW(1)
219.  DO 391 J=1,6
220.  391 MW(100-J)=MW(1)
221.  392 CONTINUE
222.  390 FORMAT (F12.1)
223.  IF (100/100 L65 DRY ASH AND COMPONENT)
224.  CONTINUE
225.  100000 FORMAT (1, MW CALCULATION)
226.  WRITE (JOUT,10080) MW(1)

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COLLV2

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227. 10000 FORMAT (2X,04.1)
228. 400 READ (5,*) IC
229. IF (IC.EQ.1) GO TO 400
230. IF (IC.EQ.1) GO TO 420
231. WRITE (JOUT,10000)
232. 10000 FORMAT (' ENTER MHV AS BTU/LB COAL')
233. READ (5,*) MHV
234. 420 MHV=MHV*10
235. IF (MHV.EQ.0) GO TO 440
236. IF (MHV.EQ.1) GO TO 421
237. WRITE (JOUT,10000)
238. 2420 IF (MFUEL.EQ.0) GO TO 2427
239. GO TO 2426
240. WRITE (JOUT,2420) 1,OFUEL(1,1),OFUEL(2,1),OFUEL(1,1),
241. * 1,OFUEL(1,1),OFUEL(2,1),OFUEL(1,1),OFUEL(1,1),
242. 2424 FORMAT (14,F10.4,F10.3,1X,A3,512X,A2,2X,F8.4)
243. 2426 CONTINUE
244. 2427 WRITE (JOUT,10052)
245. 2423 KOUT=0
246. READ (5,*) KOUT
247. IF (KOUT.EQ.0) GO TO 2422
248. IF (KOUT.EQ.0) GO TO 430
249. IF (KOUT.EQ.1) GO TO 2439
250. WRITE (JOUT,10054)
251. 2424 LN=0
252. READ (5,*) LN
253. IF (LN.EQ.0) GO TO 2428
254. IF (KOUT.EQ.1) GO TO 2432
255. C
256. DELETE
257. IF (LN.EQ.0) GO TO 2431
258. DO 2429 J=1,6
259. OFUEL(J,1)=OFUEL(J,1)
260. 2429 OFUEL(J,1)=OFUEL(J,1)
261. 2430 OFUEL(J,1)=OFUEL(J,1)
262. 2431 MFUEL=MFUEL-1
263. GO TO 2420
264. C
265. ALTER
266. 2432 NI=LN
267. GO TO 2436
268. C
269. 2434 MFUEL=MFUEL+1
270. NI=MFUEL
271. C
272. 2436 WRITE (JOUT,10060)
273. 10060 FORMAT (' TYPE LBS/LB COAL, TEMPERATURE ',
274. * '(DEG F) AND STATE AND COMPONENT')
275. DO 2438 J=1,6
276. OFUEL(J,NI)=0
277. 2438 OFUEL(J,NI)=0
278. OFUEL(J,NI)=0
279. READ (5,*) OFUEL(1,NI),OFUEL(2,NI),OFUEL(1,NI),
280. * 1,OFUEL(1,NI),OFUEL(2,NI),OFUEL(1,NI),OFUEL(1,NI),
281. GO TO 2420
282. 2421 CONTINUE
283. C

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COLCV2

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284. WRITE (JOUT,10,2)
285. 10092 FORMAT (' TYPE OTHER FUEL COMPONENTS')
286. X ' TYPE LBS/LB COALT TEMPERATURE'
287. X ' (DEG F) AND STATE AND COMPONENT'
288. NI=1
289. 422 WRITE (JOUT,10094)
290. 10094 FORMAT (5X,'EXAMPLE U-31 100. 2. 0. 0. 1. 7. 7')
291. 423 DO 424 J=1,6
292. 10FUEL(J,NI)=2H
293. 424 OFUEL(J,1,NI)=0.
294. 425 OFUEL(J,2,NI)=0.
295. 426 READ (5,9) OFUEL(1,NI),OFUEL(2,NI),OFUEL(1,NI)
296. X 10FUEL(J,NI),OFUEL(J,2,NI),J=1,51
297. IF (OFUEL(1,NI)) 427,428,427
298. 427 NI=NI+1
299. GO TO 423
300. 428 MFUEL=NI-1
301. 430 MCR=0.
302. DO 434 I=1,MFUEL
303. DO 432 J=1,5
304. IF (10FUEL(J,1,NI)) 435
305. IF (10FUEL(J,2,NI)) 435
306. 432 CONTINUE
307. MCR=OFUEL(1,NI)
308. IF (1,1,0) 435
309. DO 433 NI=1,13
310. VI=OFUEL(NI,1)
311. OFUEL(NI,1)=OFUEL(NI,1)
312. OFUEL(NI,2)=1
313. 433 CONTINUE
314. 434 CONTINUE
315. 435 CCR=0.
316. DO 438 I=1,MFUEL
317. DO 436 J=1,5
318. IF (10FUEL(J,1,NI)) 439
319. IF (10FUEL(J,2,NI)) 439
320. 436 CONTINUE
321. CCR=OFUEL(1,NI)
322. GO TO 440
323. 438 CONTINUE
324. 440 IF (JOP(1,NI)) 441,441,441
325. C READ IN OXIDIZER TEMPERATURE
326. 442 WRITE (JOUT,10,100)
327. 10100 FORMAT (' TYPE OXIDIZER TEMPERATURE IN DEG F')
328. 450 READ (5,1) OTEMP
329. 450 IF (JOP(1,NI)) 441,441,441
330. C READ IN OXIDIZER COMPONENTS
331. WRITE (JOUT,10,110)
332. 10110 FORMAT (' TYPE OXIDIZER COMPONENTS')
333. X ' TYPE LBS/100 LBS OXIDIZER AND COMPONENT'
334. NI=1
335. 452 WRITE (JOUT,10,112)
336. 10112 FORMAT (5X,'EXAMPLE 95.0 0.0 2. 7. 7')
337. 453 DO 454 J=1,5
338. 10XID(J,NI)=2H
339. 454 OXID(J,1,NI)=0.
340.

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COLCV2

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341.      OXIDIL,NI=0.
342.      READ 15,01 OXIO(1,NI),
343.      * 11OXID(1,NI),OXID(1,NI),J=1,5)
344.      IF 1OXID(1,NI) 456,460,456
345.      456 WT=NI*1
346.      GO TO 453
347.      460 NOXIO=NI-1
348.      DO 464 I=1,NOXIO
349.      00 462 J=1,5
350.      IF 11OXID(I,1),EQ,102(J) 60 TO 464
351.      IF 1OXID(I,1),EQ,02(J) 60 TO 464
352.      462 CONTINUE
353.      IF 11,EQ,1) 60 TO 470
354.      DO 463 K=1,1)
355.      71=OXID(I,K,1)
356.      OXID(K,1)=OXID(I,1)
357.      OXID(I,1)=71
358.      463 CONTINUE
359.      GO TO 470
360.      464 CONTINUE
361.      470 CONTINUE
362.      RETURN
363.      END

```

END FTM 991 IBANK 1226 DBANK 370 COMMON

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A-22

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56.      A26 IF JICCR1.A26.
57.      DO 978 I=1,MFUEL
58.      DO 976 J=1,5
59.      IF (IOFUEL(J,1),NE,ICC(J)) 60 TO 978
60.      IF IOFUEL(J,2),NE,ICC(J)) 60 TO 978
61.      976 CONTINUE
62.      OFUEL(I,J)=ICCR
63.      CCR=TCGR
64.      60 TO 979
65.      978 CONTINUE
66.      CALL ERROFF
67.      979 IF (IPER) 980.
68.      PER=IPER
69.      990 CONTINUE
70.      NREAC=0
71.      C      COMPUTATION FOR COAL CARD
72.      SINGT=COAL(1)*(1.-PER)
73.      SCOAL=COAL(1)
74.      COAL(1)=COAL(1)*PER
75.      SUM=0.
76.      N=NREAC+1
77.      NS=N
78.      DO 982 I=1,5
79.      982 SUM=SUM+COAL(I)
80.      DO 984 I=1,5
81.      984 ANUMIN(I)=ICCAL(I)/SUM*100.
82.      SUM=0.
83.      DO 986 I=1,5
84.      986 SUM1=SUM1+ANUMIN(I)
85.      986 SUM1=SUM1+ANUMIN(I)
86.      DO 988 I=1,5
87.      988 ANUMIN(I)=ANUMIN(I)/SUM1*100.
88.      C      CREATE COAL CARD
89.      DO 994 I=1,5
90.      DECODE (9,996,ICCAL(I)) NAME(N,I)
91.      996 FORWAT (A6)
92.      994 CONTINUE
93.      NAMEIN,61=N
94.      ANUMIN,61=0.
95.      C      COMPUTE COAL/FUEL RATIO
96.      CSUM=0.
97.      DO 998 I=1,MFUEL
98.      CSUM=CSUM+OFUEL(I,1)
99.      CF=100*CF/CSUM
100.      PECNIN=CF*SUM/100.
101.      MOLEIN=1W
102.      FZIN=1MS
103.      RTENPIN=ICTEMP-32.1/1.8*273.15
104.      FORWAT (A6)
105.      DEMSUM=0.
106.      NREAC=NREAC+1
107.      C      CREATE INERT CARBON CARD
108.      IF (PER-1.) .50N.
109.      N=NREAC+1
110.      DO 1000 I=1,6
111.      NAMEIN,I=6H
112.      1000 ANUMIN,I=0.

```

```
113. NAME(IN,1)=IC
114. ANUMIN,1=1.
115. PECUTIN=CF*5INR1/100.
116. MOLE(IN)=JM
117. ENTWIN=60
118. NAME(IN,6)=2MOD
119. FZ(IN)=IWS
120. RTEMPIN=RTEMPINSI
121. FOR(IN)=IMV
122. DENGIN=0.
123. NREAC=NREAC+1
124. C CREATE OTHER COAL COMPONENTS CARDS
125. 508 IF INCONC=0.07 60 TO 520
126. N=NREAC
127. DO 508 I=1,NCONC
128. DO 506 J=1,5
129. DECODE IN,496,ICOMP(J,I),NAMEIN(I,J)
130. 506 ANUMIN(I,J)=CCOMP(J,I,1)*CF/100.
131. PECUTIN(I)=CCOMP(I,1)*CF/100.
132. MOLE(IN,I)=JM
133. DECODE IN,496,ICOMP(I,1) IFAZ(IN,I)
134. ENTWIN(I)=0.
135. NAME(IN,I,6)=2MOD
136. ANUMIN(I,6)=0.
137. RTEMPIN(I)=CTEMP-32.17/1.8*273.15
138. FOR(IN,I)=IMV
139. DENGIN(I)=0.
140. 508 CONTINUE
141. 520 NREAC=NREAC+NCONC
142. C CREATE CARDS FOR ASH COMPONENTS
143. NAME(IN,1)=IC
144. SUMZ=0.
145. IF INASH=0.01 60 TO 590
146. ASHF=CF*PROX131/100.
147. DO 522 I=1,NASH
148. 522 SUMZ=SUMZ+ACOMP(I,1)
149. DO 524 I=1,NASH
150. DO 526 J=1,5
151. DECODE IN,496,ICOMP(J,I),NAMEIN(I,J)
152. ANUMIN(I,J)=ACOMP(J,I,1)
153. PECUTIN(I)=ACOMP(I,1)*ASHF1/SUMZ
154. MOLE(IN,I)=IM
155. FZ(IN,I)=IWS
156. ENTWIN(I)=0.
157. NAME(IN,I,6)=2MOD
158. ANUMIN(I,6)=0.
159. RTEMPIN(I)=CTEMP-32.17/1.8*273.15
160. FOR(IN,I)=IMV
161. DENGIN(I)=0.
162. 528 CONTINUE
163. 590 NREAC=NREAC+NASH
164. C COMPUTE ENTHALPY FOR COAL
165. FES2=FES2+ASHF/(SUMZ*CF)
166. HHV=(HHHV-14405.7*5INR1/100.)/1.8*(100./SUM1+100./SUM1)*100.
167. FES2=(100./1.8*(100./SUM1+100./SUM1)*100.)/SUM1+4FES2
168. HFI=-ANUMINS,1)*94051.8-0.5*ANUMINS,2)*48317.4
169. X -ANUMINS,5)*70960.-FES2*Cal97650.
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COLCV3

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1 227. PECWTIN(I)=OXID(I,I)/SUM3
1 228. MOLE(I,I)=IM
1 229. FZIN(I,I)=IMG
1 230. ENTHIN(I,I)=O.
1 231. NAME(I,I)=2400
1 232. ANUM(I,I)=O.
1 233. ATEMP(I,I)=1000+200+10+200+15
1 234. FORIN(I,I)=IMO
1 235. DENS(I,I)=100.
1 236. 570 CONTINUE
1 237. 590 NAME=NAME+NOXID
238. C SAVE COAL DATA
239. COAL(I,I)=6000
240. NEWIND IC
241. WRITE (IC) NAME,CF,IMMV,MCRA,PER,CCR
242. WRITE (IC) CTEMP,OTEMP
243. WRITE (IC) PROX,TCORL,TCORLTT,COALTT,I=1,5,PER,IC,MM
244. WRITE (IC) NCOAL,NASH,MFUEL,NOXID
245. WRITE (IC) TTECOMP(I,J),CCOMP(I,J),I=1,61,J=1,NCOAL,I,
246. X (ACOMP(I,J),IACOMP(I,J),ACOMP(I+1,J),I=1,5),J=1,NASH,I,
247. X (OFUEL(I,J),OFUEL(2,J),OFUEL(I+2,J),I=1,5),J=1,NFUEL,I,
248. X (OFUEL(I+1,J),OFUEL(I+2,J),I=1,5),J=1,NFUEL,I,
249. X (OXID(I,J),IOXID(I,J),OXID(I+1,J),I=1,5),J=1,NOXID,I
250. C WRITE OUT REACTANT FILE
251. WRITE (IC) NAME,CF
252. DO 610 I=1,NREAC
253. WRITE (IC) NAME(I,I),ANUM(I,I),J=1,61,PERCUT(I,I),MOLE(I,I),
254. X ENTH(I,I),NAME(I,61),ANUM(I,61),AZ(I,I),ATEMP(I,I),OX(I,I),DENS(I,I)
255. 610 CONTINUE
256. TWOFICE IC
257. 680 CONTINUE
258. C FILL IN PLOT DATA
259. IF (IPLT.EQ.O) RETURN
260. ST=O.
261. IF (MCRA) 682.
262. ST=OFUEL(2,I)
263. 682 CONTINUE
264. DO 700 I=1,I3
1 265. PLOT(12,I)=MCR
1 266. PLOT(13,I)=PER
1 267. PLOT(14,I)=CCR
1 268. PLOT(15,I)=CF
1 269. PLOT(16,I)=COAL(I,I)
1 270. PLOT(17,I)=COAL(2,I)
1 271. PLOT(18,I)=COAL(3,I)
1 272. PLOT(19,I)=COAL(4,I)
1 273. PLOT(110,I)=COAL(5,I)
1 274. PLOT(11,I)=PROX(I,I)
1 275. PLOT(112,I)=CTEMP
1 276. PLOT(113,I)=MMV
1 277. PLOT(114,I)=ST
1 278. PLOT(115,I)=OXID(I,I),I
1 279. PLOT(116,I)=OTEMP
1 280. 700 CONTINUE
281. RETURN
282. END

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END IN 1231 2BANK 1262 DRAWK 958 COMMON

AMC 5 CPMS

DATE 051981

PAGE 6

CPMS

3PTM,5 CPMS,CPMS

FTM 091205/10/81-16:3113,1

1. SUBROUTINE CPMS

2. C
3. E CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES
4. C

5. INTERCAL SUB-SUBLET

6. INCLUDE SPECPR.LIST

7. COMMON /SPECPR/ N150, J31, CEMEN150, S1150, MO150, DELM150, SUB150, J1, IUSE1150, SLN150, TEMP150, 2)

8. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

9. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

10. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

11. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

12. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

13. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

14. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

15. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

16. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

17. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

18. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

19. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

20. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

21. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

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27. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

28. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

29. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

30. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

31. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

32. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

33. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

34. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

35. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

36. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

37. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

38. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

39. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

40. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

41. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

42. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

43. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

44. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

45. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

46. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

47. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

48. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

49. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

50. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

51. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

52. COMMON /MISC/ ENM, SUMN, TT, SO, ATOM13, 101, LLMT(25), 80(25),

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2 113. C CONVERGENCE TEST
2 114. IF (LE-10-AND- (FM-FB,0:ST-OUT) 80 TO 205
2 115. RMOC(MPT) = 0.01
2 116. IF (C(MPT) .LE. 0.01) GO TO 60
2 117. CM(MPT) = CP(MPT)/IC(MPT) - 0.0001/AM1
2 118. VMOC(MPT) = UN/SORTINGROCM(MPT)OTIT(I)/AM1
2 119. GO TO 150
2 120. RMOC(MPT) = 0.
2 121. VMOC(MPT) = 0.
2 122. 150 R = 0
2 123. IF (IP .EQ. MP .AND. IT .EQ. MT .OR. IT .LE. 0.01) 80 TO 860
2 124. R = MPT
2 125. IF (MPT .NE. IT) 80 TO 870
2 126. C OUTPUT
2 127. 900 WRITE(JOUT,97
2 128. 5 FORMAT(I1,97,96,DETONATION PROPERTIES OF AN IDEAL REACTING GAS )
2 129. CALL OUT1
2 130. WRITE(JOUT,98)
2 131. 96 FORMAT(13M UNFURNED GAS//)
2 132. FM(1) = F13
2 133. FM(2) = F13
2 134. WRITE(JOUT,FM1) F13,FB,FB,IPUR(I), J = 1,MPT)
2 135. FM(1) = F13
2 136. WRITE(JOUT,FM1) F13,FB,IPUR(I),J=1,MPT)
2 137. WRITE(JOUT,FM1) FM,FB,INIT(J),J=1,MPT)
2 138. DO 56 J = 1,MPT
2 139. V(J) = 0.01
2 140. 56 SORTINGROCM(I)OTIT(I)/AM1
2 141. FM(1) = 1.00
2 142. WRITE(JOUT,FM1) FM,FB,INIT(J),J=1,MPT)
2 143. FM(1) = 1.00
2 144. WRITE(JOUT,FM1) FM,FB,INIT(J),J=1,MPT)
2 145. WRITE(JOUT,FM1) FM,FB,INIT(J),J=1,MPT)
2 146. FM(1) = 0.01
2 147. WRITE(JOUT,FM1) FSV,FVEL,ISOMVEL(I),J=1,MPT)
2 148. WRITE(JOUT,50)
2 149. 50 FORMAT(13M UNFURNED GAS//)
2 150. FM(1) = 0.01
2 151. CALL OUT2
2 152. WRITE(JOUT,98)
2 153. 60 FORMAT(22M DETONATION PARAMETERS //)
2 154. FM(1) = 1.00
2 155. 70
2 156. 70 SORTINGROCM(I)OTIT(I)/AM1
2 157. PCPI(J) = IT(I)/INIT(I)
2 158. WRITE(JOUT,FM1) FSV,FVEL,ISOMVEL(I),J = 1,MPT)
2 159. WRITE(JOUT,FM1) FSV,FVEL,ISOMVEL(I),J = 1,MPT)
2 160. WRITE(JOUT,FM1) FSV,FVEL,ISOMVEL(I),J = 1,MPT)
2 161. DO 13 J = 1,MPT
2 162. V(J) = 0.01
2 163. FM(1) = 0.01
2 164. WRITE(JOUT,FM1) FM,FB,IPUR(I), J = 1,MPT)
2 165. WRITE(JOUT,FM1) FM,FB,IPUR(I), J = 1,MPT)
2 166. WRITE(JOUT,FM1) FM,FB,IPUR(I),J=1,MPT)
2 167. FM(1) = 0.01
2 168. WRITE(JOUT,FM1) FUD,FVEL,ISOMVEL(I),J=1,MPT)
2 169. COL = TRUE.
2 170.

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DETON

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2 170. CALL OUT
2 171. IF IN .EQ. 0 .AND. IOF .EQ. NOF) GO TO 1000
2 172. IDEBUG = IDEBUG+13
2 173. WRITE(JOUT,868)
2 174. 868 FORMAT(1M1)
2 175. NPT = 0
2 176. 870 NPT = NPT+1
2 177. IF IN .EQ. 1) K = -1
2 178. CALL SAVE
2 179. WRITE(JOUT,868)
2 180. 902 CONTINUE
2 181. IF IOF .GE. NOF) GO TO 1000
2 182. IDEBUG = IDEBUG+13
2 183. GO TO 7
2 184. 1000 TP = .FALSE.
2 185. RETURN
2 186. END

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END FTM 614 IRANK 616 DBANK 1437 COMMON

END P EQU8M


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1 53. IUSE(JJ) = 0
1 54. 499 CONTINUE
55. 33 IF (MPT.EQ.1) AND (NOT=SHOCK) WRITE(JOUT,244) (LLMT(I),I=1,L)
56. 244 FORMAT (NOPT,1X,ANI)
57. C BEGIN ITERATION
58. 43 IF (IC) GO TO 1171
59. IF (NOT=CONVG) GO TO 62
60. SUM = CN
61. IF (JSOL.EQ.0) GO TO 62
62. ENSOL = EN(JSOL,MPT)
63. EN(JSOL,MPT) = EN(JSOL,MPT) + EN(JL3,MPT)
64. IUSE(JL3) = -IUSE(JL3)
65. IOL = IOL + 1
66. DLVTP(MPT) = 0.
67. CPRINTL = 0.
68. GAMMA(MPT) = 0.
69. LOGV = .TRUE.
70. 62 CALL MATRIX
71. NUMB = IOL - IINUMB
72. IOL = IOL + 1
73. IF (NOT=CONVG) GO TO 67
74. IF (LOGV.AND.JSOL.EQ.0) GO TO 63
75. DO 102 I=1,L
76. 102 PROM(I) = G(IOL,I)
77. IF (L.NOL) LOGV = 0.10
78. C LOGV = .TRUE. -- SET UP MATRIX TO SOLVE FOR DLVTP
79. 63 G(IOL,IOL) = CN
80. J = IOL - 1
81. DO 777 I=1,J
82. 777 G(I,IOL) = G(I,I)
83. 67 IF (NOT=WRITE) GO TO 72
84. WRITE(JOUT,73) (I,I=1,J)
85. 772 FORMAT (11M) ITERATION ,13,6X,7MMATRIX (/)
86. DO 911 I=1,IMAT
87. 911 WRITE(JOUT,73) (G(I,I),I=1,IMAT)
88. 72 IF (CONVG) IMAT=IMAT+1
89. J = IMAT
90. C END CROSS
91. IF (J.NE.IMAT) GO TO 774
92. IF (NOT=WRITE) GO TO 773
93. WRITE(JOUT,73) (LLMT(I),I=1,L)
94. 373 FORMAT (7M) 19(AN,10X)
95. WRITE(JOUT,73) (I,I=1,IMAT)
96. 73 FORMAT (10X)
97. 773 IF (NOT=CONVG) GO TO 85
98. IF (NOT=LOGV) GO TO 174
99. IF (JL3.NE.0) EN(JSOL,MPT)=ENSOL
100. GO TO 171
101. 174 SUM = 0.
102. DO 175 J=1,L
103. 175 SUM = SUM + PROM(J) * X(J)
104. DLVTP(MPT) = 1.0 * G(IOL,IOL) / (ENM-SUM/ENM - X(IOL))
105. CPRINTL = G(IOL,IOL)
106. DO 176 J=1,IOL
107. 176 CPRINTL = CPRINTL - G(IOL,J) * X(J)
108. LOGV = .TRUE.
109. GO TO 62

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EOLDRM

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110. C SINGULAR MATRIX
111. 774 IF (.NOT. CONV) GO TO 775
112. C IF (ISING) SINGULAR ONCE
113. C IF (IC) SINGULAR TWICE
114. WRITE(JOUT,172)
115. 172 FORMAT(28X'DEPRIVATIVE MATRIX SINGULAR')
116. IC = .TRUE.
117. GO TO 1171
118. 775 IF (.NOT. MP.OP.NPT;ME.1 OR MC.E.O.O.R.O.T.T.GT.100) GO TO 071
119. WRITE(JOUT,874)
120. 874 FORMAT(6X'LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
121. BEEN INCLUDED ON AN INSERT CARD, RESTART')
122. GO TO 873
123. 871 WRITE(JOUT,74)
124. 74 FORMAT(16X'SINGULAR MATRIX')
125. IF (IC) GO TO 873
126. IF (ISING) GO TO 997
127. NZERO = 0
128. 966 DO 970 JJ = 1, NS
129. IF (IUSE(JJ)) 970, 968, 967
130. 967 IF (EN(JJ,NPT)) 969, 873, 969
131. 968 IF (EN(JJ,NPT)) 87. 0.0) GO TO 969
132. EN(JJ,NPT) = 1.0E-6
133. ENL(JJ) = -13.015511
134. GO TO 970
135. 969 NZERO = NZERO+1
136. 970 CONTINUE
137. IF (.NOT. IUSE) GO TO 971
138. IC = .FALSE.
139. GO TO 83
140. 971 ISING = .TRUE.
141. WRITE(JOUT,776)
142. 776 FORMAT(10X'RESTART')
143. GO TO 83
144. 997 IF (NZERO.NE.L-1. OR.EORAT.GI.1.200Q1. OR.EORAT.LT..99999) GO TO 873
145. ENN = 0
146. ENN = 0
147. DO 83 I=1,L
148. JJ = 0
149. DO 80 J=1,NS
150. IF (EN(J,NPT).EQ. 0.0. OR. A(I,J).EQ. 0.0) GO TO 80
151. IF (JJ.NE. 0) GO TO 83
152. 80 CONTINUE
153. ENN = ENN+1
154. EN(JJ,NPT) = PUT(I7A11,JJ)
155. 83 CONTINUE
156. IF (ENN.LT.NTZERO) GO TO 873
157. CONV = .TRUE.
158. IC = .TRUE.
159. HSUM(NPT) = 0.
160. DO 84 J=1,NS
161. IF (EN(J,NPT).LE. 0.0) GO TO 84
162. ENN = ENN+1
163. ENL(JJ) = ALQ(EN(J,NPT))
164. HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H(N(J)
165. 84 CONTINUE
166.

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COLBPM

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167. 7M = ALOG(PP/ENN)
168. GO TO 43
169. AS ITNUMB = ITNUMB-1
170. IF ITNUMB .LT. 301 CRITV = CRITV + 2.50E-7
171. 2 OBTAIN CORRECTIONS TO THE ESTIMATES
172. JJ = 1 + 1
173. IF (VOL) X(102) = X(101)
174. IF (PT) X(102) = 0.
175. DUNT = X(102)
176. SUM = X(101)
177. IF (NOT VOL) GO TO 97
178. X(101) = 0.
179. SUM = -DUNT
180. 97 DO 101 J=1,MS
181. IF (IUSE(J)) 101,98,100
182. 98 DELN(J) = HO(J)*DUNT-HO(J)*S(J)-ENLN(J)-TM*SUM
183. DO 99 I = 1,L
184. 99 DELN(I) = DELN(J) + A(I,J)*X(I)
185. GO TO 101
186. 100 DELN(J) = X(J)
187. JJ = JJ + 1
188. 101 CONTINUE
189. AMBDA = 1.
190. AMBDA1 = 1.
191. SUM = X(101)
192. IF (SUM .LT. 0.1) SUM = -SUM
193. IF (DUNT .GT. SUM) SUM = DUNT
194. IF (DUNT .LT. -SUM) SUM = -DUNT
195. 99 IUSE(J) = 1.
196. IF (IUSE(J)) .GT. 0.1 GO TO 917
197. IF (EN(J,NPT)) .GT. 0.0 .AND. DELN(J) .GT. SUM SUM = DELN(J)
198. IF (EN(J,NPT)) .GT. 0.0 .AND. DELN(J) .LT. -SUM SUM = -DELN(J)
199. SUM1 = 1-9.212-ENLN(J) ENL1/(DELN(J)-X(101))
200. IF (SUM1 .LT. 0.1) SUM1 = -SUM1
201. IF (SUM1 .LT. AMBDA1) AMBDA1 = SUM1
202. 917 CONTINUE
203. IF (SUM .GT. 2.1) AMBDA = 2./SUM
204. IF (AMBDA1 .LT. AMBDA) AMBDA = AMBDA1
205. IF (NOT RITE) GO TO 111
206. WRITE(JOUT,923) IT,ENN, ENL,PP,FM,AMBDA
207. 923 FORMAT (3HOUT=,E15.8,6H ENN=,E15.8,7H FNNL=,E15.8,5H PP=,E15.8,
208. 1.9H - LN P/N=E15.8,6H AMBDA=E15.8)
209. IF (VOL) WRITE(JOUT,1924) VLMINPT)
210. 1924 FORMAT(10H VOLUME=,E15.8,2HGET)
211. WRITE(JOUT,924)
212. 924 FORMAT(10H I=,2HNI=,12H,5H N=,9H,9HDEI LN W=,10H,4HMM/RT,9H,4H50/
213. 1R,12H,6H-GO/PT,9H,5H-G/RT)
214. DO 926 J=1,MS
215. FNEG1 = FNEG1-HO(J)
216. FNEG2 = FNEG1
217. IF (IUSE(J)) FNEG2 = FNEG2-ENLN(J)-TM
218. 926 WRITE(JOUT,925) SUB(J,1),SUB(J,2),SUB(J,3),EN(J,NPT),ENLN(J),
219. 925 A DELN(J),HO(J),S(J),FNEG1,FNEG2
220. 925 FORMAT (1X,34H,7E15.6)
221. WRITE(JOUT,110)
222. 110 FORMAT(1H0)
223. C APPLY CORRECTIONS TO ESTIMATES

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• EOLN0079
• EOLN0080
• EOLN0081

• EOLN0084

• EOLN0089
• EOLN0090

• EOLN0096

ORIGINAL PAGE IS
OF POOR QUALITY

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224. 111 SUM = 0.
225. DO 113 J=1,N5
226. IF (IUSE(J)) 113,112,114
227. 112 ENL(J)=ENL(J)+AMDA*DEL(J)
228. ENL(NPT)=0
229. IF (ENL(NJ)+10.020810.LE.ENL) GO TO 113
230. ENL(NPT)=EXP(ENL(NJ))
231. SUM=SUM+ENL(NPT)
232. DO 113 J=1,N5
233. 113 ENL(NPT)=ENL(NPT)+AMDA*DEL(NJ)
234. 113 CONTINUE
235. SUM=SUM
236. IF (111-00-113)
237. TLM=TLN+AMDA*DLMT
238. PT=EXP(TLM)
239. JS1=1
240. CACL CPMS
241. 115 IF (VOL) GO TO 2115
242. ENL=ENL+AMDA*PT*1000
243. ENN=EXP(ENL)
244. DO 115 J=1,N5
245. 2115 ENN=SUM
246. ENNL=ALOG(ENN)
247. PP=RV*PT*ENN/VLM(NPT)
248. 1115 IM=ALOG(PP/ENN)
249. IF (IM) 116,117,118
250. C CHECK ON REMOVING IONS
251. DO 116 J=1,N5
252. IF (IALL(J).EQ.0.) GO TO 1116
253. IF (IENL(NPT)*GT.0.) GO TO 116
254. 1116 CONTINUE
255. DO 1110 J=1,N5
256. 1110 IF (IALL(J).NE.0.0) IUSE(J)=-10000
257. C=-1
258. 101=101-1
259. GO TO 43
260. C 116 IF 111 FROM 116 TO 13
261. IF (AMDA*LT.1.) GO TO 43
262. SUM=(ENN-SUM)/ENN
263. IF (SUM*LT.0.) SUM=-SUM
264. IF (SUM*GT.0.) CRITI GO TO 43
265. DO 130 J=1,N5
266. IF (IUSE(J).LT.0.) GO TO 130
267. AA=DEL(NJ)/SUM
268. IF (AA*LT.0.) AA=-AA
269. IF (IUSE(J).EQ.0.) AA=AA*ENL(NPT)
270. IF (IUSE(J).EQ.0.) AA=AA*ENL(NPT)
271. IF (TA*GT.0.) CRITI GO TO 43
272. 130 CONTINUE
273. C CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
274. TOT(NPT)=0
275. SSUM(NPT)=0
276. DO 183 J=1,N5
277. IF (IUSE(J).LT.0.) GO TO 183
278. IOL(NPT)=IOL(NPT)+ENL(NPT)
279. SS=SS(J)
280. IF (IUSE(J).EQ.0.) SS=SS-ENL(NJ)-TM

```

SSUMINP13 = SSUMINP13ASSEMBLY.MPI1
EOLNO136

201. 103 CONTINUE
202. IF (NOT SP OR NPT EQ 1) GO TO 13
203. SS = SSUMINP1 - 50
204. IF (SS LT (-D.00005) OR SS GT D.00005) GO TO 43
205. IF (IRITE) WRITE(JOUT,1183) SS
206. 11P3 FORMAT(12MODELTA S/P =,F15.0)
207. 13 CONVE = .TRUE.
208. IF (ITV .LT. TLOW OR ITV .GT. THIGH) WRITE(JOUT,306) IT, NPT
209. 306 FORMAT(12MODELTA TEMPERATURE =,F12.4, 26H IS OUT OF RANGE FOR POINT, I5) . EOLNO119
210. IF (ITVMB .LT. 0) GO TO 160
211. WRITE(JOUT,923) NPT
212. 973 FORMAT (75X,69H100 ITERATIONS DID NOT SATISFY THE CONVERGENCE REQ
213. 974 EOR MAT (5X, 2809 TEMPERATURE =,F12.4, 26H IS OUT OF RANGE FOR POINT, I5) . EOLNO117
214. IF (1.NOT.MP OR NPT.NE.1 OR NC.EQ.0 OR T.1.GT.100.1) GO TO 873
215. WRITE(JOUT,923) NPT
216. TT = T(11)
217. RETURN
218. C
219. CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
220. 160 IF (NC.EQ.0) GO TO 143
221. SIZEF = 0.
222. INC = 0
223. DO 170 J = 1, NS
224. IF (IUSE(J).EQ.0 OR IUSE(J).EQ.-10000) GO TO 170
225. INC = INC + 1
226. IF (IRITE) WRITE(JOUT,100) ISUB(J,1), I2, 1, TEMPIINC, 1, TEMPIINC, 2, 1
227. 100 IF (TEMP(J).GT.10.3) SHIUSE = 1, 10, 1, 1, 1
228. 100 IF (TEMP(J).GT.10.3) SHIUSE = 1, 10, 1, 1, 1
229. 100 IF (TEMP(J).GT.10.3) SHIUSE = 1, 10, 1, 1, 1
230. JSOL = 0
231. JLT0 = 0
232. 107 101 = 101 - 1
233. ENTJ,NPT = 0.
234. GO TO 166
235. 108 NG = 1
236. IF (IUSE(J).EQ.-IUSE(J,1)) GO TO 154
237. IF (J EQ 1 OR IUSE(J).NE. -IUSE(J-1)) GO TO 193
238. NG = -1
239. 154 JMB = J + NG
240. IF (IEMJNG, NPT).LT.0.1 GO TO 170
241. TMELT = TEMPIINC + 1
242. IF (ITMELT.EQ. TEMPIINC*NG, 2) GO TO 148
243. TMELT = TEMPIINC, 2
244. IF (ITMELT.EQ. TEMPIINC*NG, 1) GO TO 147
245. WRITE(JOUT,154) 1
246. 156 FORMAT(12MODELTA TEMPERATURE =,F12.4, 26H IS OUT OF RANGE FOR POINT, I5) . EOLNO117
247. C JMW SPECIES A SOLID (IEM=0), IJ*KGITH SPECIES A LIQUID (IEM IS +)
248. 157 IF (ITV .GT. TMELT) OR (ITP .AND. TT .EQ. TMELT) GO TO 169
249. IF (ITP .OR. 1) .LT. TMELT - 150.0) GO TO 1165
250. JSOL = J
251. JLT0 = JMB
252. GO TO 159
253. C JMW SPECIES A LIQUID (IEM=0), IJ*KGITH SPECIES A SOLID (IEM IS +)
254. 158 IF (ITV .LT. TMELT) OR (ITP .AND. TT .EQ. TMELT) GO TO 169

EOLM

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1 338. IF (TP .OR. IT .GE. TMELT + 150.0) GO TO 1165
1 339. JSOL = JNG
1 340. DELT = 0
1 341. 159 TLM = ALOG (TMELT)
1 342. IT = TMELT
1 343. EN(JNG,MPT) = 5 * EN(JNG,MPT)
1 344. EN(JNG,MPT) = EN(JNG,MPT)
1 345. GO TO 165
1 346. C- WRONG PHASE INCLUDED FOR T INTERVAL SWITCH EN
1 347. 1165 EN(J,MPT) = EN (JNG, MPT)
1 348. 105E(1) = -105E(1)
1 349. IUSE (JNG) = -IUSE(JNG)
1 350. EN(JNG,MPT) = 0.
1 351. WRITE(JOUT,161) (SUBJ,J,I, I = 1,3), (SUBJ,J,I), I = 1,3)
1 352. 161 FORMAY 10X,22PHASE CHANGE, REPLACE 3PH, ON WITH 3AW)
1 353. GO TO 40
1 354. 153 IF (IT,LT,TEMP(1), .AND,TEMP(1),NE, TLOW) GO TO 169
1 355. IF (IT,GT,TEMP,INC,20) GO TO 169
1 356. SUM = 0.
1 357. DO 167 J = 1,4
1 358. 167 SUM = SUM + ALL(J)X(1)
1 359. DELF = MO(J)-S(J)-SUM
1 360. IF (RTE) WRITE(JOUT,168)DELF,SIZEF
1 361. 168 FORMAY (17M GO-SUM(RJOP)) =E15.7,10X,1AMPREVIOUS DELTA 6 =,E15.7)
1 362. IF (DELF .GE. SIZEF .OR. DELF .GE. 0.1) GO TO 169
1 363. SIZEF = DELF
1 364. JOELF = J
1 365. 169 IF (INC.EQ.MC) GO TO 1160
1 366. 170 CONTINUE
1 367. 1160 IF (SIZEF.EQ.0.1) GO TO 143
1 368. 165 JOT = 101 + 1
1 369. WRITE(JOUT,136) (SUBJ,J,I, I = 1,3)
1 370. 136 FORMAY 10X,4HDD,3AW)
1 371. 166 JUSELJ = - JUSELJ
1 372. 40 CONVG = .FALSE.
1 373. CALL CPMS
1 374. 143 IN = NUMB
1 375. 77: FORMAY 113,14F9.3)
1 376. 77: FORMAY 113,14F9.3)
1 377. JSI = 1
1 378. IF (12.AND.CONVG) CALL CPMS
1 379. 11NUMP = 100
1 380. GO TO 43
1 381. C- CALCULATE EQUILIBRIUM PROPERTIES
1 382. 1171 OLVP(MPT) = -1.
1 383. OLVP(MPT) = 1.
1 384. OLVP(MPT) = 1.
1 385. CPP(MPT) = CPSUM
1 386. GO TO 199
1 387. 171 SUM = 0.
1 388. DO 176 J = 1,4
1 389. 176 SUM = SUM + FROM(J)X(1)
1 390. OLVP(MPT) = 2.0 * SUM / ENN * X(1)
1 391. IF (JULIO .EQ. 01) GO TO 199
1 392. IUSF(JULIO) = -IUSE(JULIO)
1 393. HSUM(MPT) = HSUM(MPT) + EN(JULIO,MPT) * MC(JULIO) - MO(JULIO)
1 394.

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EOLM0126
EOLM0128

EOLM0167
EOLM0170


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395.      IQ1 = IQ1.1
396.      GAMMAS(NPT) = -1./OLVPT(NPT)
397.      GO TO 186
398.      199 GAMMAS(NPT) = -1./OLVPT(NPT)*OLVTP(NPT**2)*ENN/C*PRINPT))
399.      196 TT(NPT) = TT
400.      ENNL = ENL
401.      PPP(NPT) = PP
402.      VLM(NPT) = RVP*ENN*PP
403.      MSUR(NPT) = MSUM(NPT)*T
404.      VM(NPT) = 1./ENN
405.      IF (.NOT. RTE) RETURN
406.      NB1 = (OUT-201)*NPT*APP(NPT), PP, TY, MSUM(NPT), SSUM(NPT), VM(NPT),
407.      1 C*PRINPT), OLVPT(NPT), OLVTP(NPT), GAMMAS(NPT), VLM(NPT)
408.      201 FORMAT (7HPOINT=13.3X, 4HPCP=13.6, 3X, 2HP=13.6, 3X, 2MT=13.6, 3X, 4H
409.      1H/R=13.6, 3X, 4HMS/R=13.6//3X, 3HNU=13.6, 3X, 5HCP/R=13.6, 3X, 6HOLVPT
410.      2=13.6, 3X, 6HOLVTP=13.6, 3X, 4HGMMAIS)=13.6, 3X, 2MT=13.6)
411.      RETURN
412.      C
413.      873 TT=0
414.      NPT = NPT-1
415.      RETURN
416.      END

```

END FTM 1957 IBANK 830 DRANK 11980 COMMON

3106.P FROZEN

FROZEN

051901 FROZEN FROZEN

FTN 001M2005/19/01-16132112.1

1. SUBROUTINE FROZEN

2. C (FROZEN COMPOSITION EXPANSION ONLY)

3. C

4. C COMMON /COMMON/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)

5. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

6. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

7. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

8. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

9. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

10. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

11. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

12. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

13. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

14. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

15. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

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51. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

52. C COMMON /COMMON/ATM,GMEZ,PAIR,ROAR,ROR,RHR

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FROZEN

DATE 051003

PAGE

2

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53.      MSURIMP12= J10SUMH
54.      GAMMASIMP12= CPSUM/ICPSUM-1./UMINF21)
55.      VIMP12= PAROTT/UMINF219991
56.      UIMP12= UMINF21
57.      DLVIMP12= -1.
58.      DLVIMP12= 1.
59.      TOTIMP12= TOTIMP12)
60.      PPIMP12= PP
61.      CPIMP12= CPSUM
62.      IF (IT.LI,110W-150,1160 TO 903
63.      IF (INC .EQ. 0) RETURN
64.      INC = 0
65.      DO 901 J = 1,NS
66.      IF (IUSE(J) .EQ. 0 .OR. IUSE(J) .EQ. - 10000) 60 TO 901
67.      INC = INC+1
68.      IF (EM(J,NEZ) .LE. 0.0) 60 TO 901
69.      IF (IT.LT.TEMP(INC,1)-50. .OR. IT.GT.TEMP(INC,2)+50.) 60 TO 901
70.      901 CONTINUE
71.      RETURN
72.      903 IT=0.
73.      NPT= NPT-1
74.      RETURN
75.      END

```

. FROZEN

END FTM 235 IRAN: 35 ORAN 10471 COMMON

JH06.P GAMEFF

GAMEFF

011155 GAMEFF, GAMEFF
 FVN 00112005/10/01-153316.1

1. SUBROUTINE GAMEFF IV, GAMMAS, A, M, M)
 2. DIMENSION A(13), GAMMAS(13), M(13), V(13)
 3. C

4. DO 50 I = 2, N

5. G = GAMMAS(I)

6. AMR = 1.0

7. IF 16 .GT. 1.01 GO TO 10

8. G = 1.0010

9. GP = G + 1.0

10. GM = G - 1.0

11. CONTINUE

12. CFA = CGAMESORT(12, 0.001, 1.0 - (1.0/AMR)) * (GM/61)/GM)

13. IF (ABS(CFA) - CFA) .LT. 5.0E-37 GO TO 30

14. IF 16 .LT. 2.01 GO TO 20

15. IF 16 .LT. 0.01 GO TO 30

16. AMR = -1.0

17. G = GAMMAS(I)

18. GO TO 10

19. GP = G + AMR * V(1) - CFA

20. IF 16 .GT. 1.01 GO TO 10

21. IF 16 .LT. 0.01 GO TO 30

22. AMR = -1.0

23. G = GAMMAS(I)

24. GO TO 10

25. GO

26. RETURN

27. END

END FIN 100 JPRNR 98 00AMH

AMG, P GAUSS

GAUSS

DATE 051001 PAGE 2

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54. 07 J = N * J
55. 0000
56. SUM = 0.0
57. IF (USE .LT. J) GO TO 51
58. 00 50 I = 0.0000
59. SUM = SUM + G(A, I, I, I)
60. 51 50 I = 0.0000
61. SUM = SUM + G(A, I, I, I)
62. 52 50 I = 0.0000
63. SUM = SUM + G(A, I, I, I)
64. 53 50 I = 0.0000
65. RETURN
66. 54 50 I = 0.0000
67. RETURN
68. END
```

END OF PROGRAM

END OF PROGRAM

END OF PROGRAM
DATE 05/10/01 16:33:00

SECTION

DATE 051901

PAGE 1

SPYING IN 200-TPP-6101-SECTION
1 OF REE TPRS.
2 0A50, 1 TPPS, 731005/3
3 0USE TPRS, 1LEWIS.
4 0A50, 1A 4:
5 0A56, 1A 8:
6 0A56, 1A 10:
7 0A56, 1A 12:

0A06, 0A 0A56

C-2

1. E1133191-18/41/50024186 N13

THE

COMMON /NO310M/

6. INCLUDE SPECIMEN LIST

[illegible]

0.7% normal weight loss

0811251-1W13

Q. N1111521AHH 5

1 MAY, 1961, 101

3

STRENGTHEN HIMSELF

INTEGER A6,BLN,F A2,FOX,OX

IF (AM(1)) .GT. 0.0 .AND. AM(1) .LT. 1.0

10.0.37. (2) MW 11

11-11-68

SUMMARY = 0.

• 0.1214M

• 9 = 1943 •

3 :
JAN 11 1966

IF(FOX(N).EQ.OX)N=1

IF .NOT .CALCH1 GO TO 15

. C IS IT IN RANGE

17. $\sin^{-1} \frac{1}{2} = \frac{\pi}{6}$

1980

00 30 1:1.5


```

3 20 30 J=1
5 20 IF (LLMT(J).EQ. NAMEIN,1) 60 TO 30
2 30 DATA J = DATA(J) + ANUMIN,1
1 56 50 IS=0
1 57 60 70 J=1,NS
2 58 IF (IUSE(J).EQ.0) 60 TO 55
2 59 IS = IS+1
2 60 IF (FAZIN).EQ. AG 60 TO 70
2 61 IF (IT.TEMP(IIS,2).AND.TEMP(IIS,2).NE.THIGH) 60 TO 70
2 62 IF (IT.LI.TEMP(IIS,1).AND.TEMP(IIS,1).NE.FLOW) 60 TO 70
2 63 60 TO 56
2 64 55 IF (FAZIN).NE. AG.AND.FAZIN.NE.BLK) 60 TO 70
2 65 56 60 60 I=1,L
2 66 60 IF (AIL(J).NE. DATA(I)) 60 TO 70
2 67 ANUMIN,6)=J
2 68 60 TO 90
2 69 70 CONTINUE
1 70 60 TO 80
1 71 90 IF (MOLES) ENJ = PECMTIN/MPIN
1 72 IF (L.MOI,MOLES) ENJ = PECMTIN/PMIN
1 73 ENJ = ENJ/ANM
1 74 IF (ENJ) ENJ = ENJ*OF
1 75 IF (NAMEIN,6).NE.ZERO) 60 TO 500
1 76 I = NS
1 77 NS = J
1 78 TLM = ALOGITT)
1 79 IF (NOT.CALCH) ENJ,NPT) = ENJ
1 80 CALL CPMS
1 81 IF (MO(J).GT..01 .AND. MO(J).LT..01) MO(J) = 0.
1 82 IF (ENJ) ENJ = 1
1 83 IF (ENJ) ENJ = 1
1 84 ENJIN) = PPAROT(HO(J)
1 85 CPM = CPM + CPSON
1 86 500 MSUBO = MSUBO + ENJIN*ENJ
1 87 NPTIN) = NPTIN*ENJIN*ENJ
1 88 900 SSURINPT) = SSURINPT) + ENJ*(IS(J) - ALOGIENJ) - TM)
1 89 77 = YSAVE
1 90 MSUBO = MSUBO/RRAP
1 91 RETURN
1 92 75 WRITE(JOUT,76)
1 93 76 FORMAT(1720X,12#REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA
1 94 11N MCALC/)
1 95 RETURN
1 96 80 WRITE(JOUT,85) N
1 97 85 FORMAT(1720X,12#REACTANT IS NOT IN THERMO DATA IN MCALC/)
1 98 RETURN
1 99 END
100

```

END FTM 356 IRANK 87 DBANK 10326 COMMON

AMOG.P LISTIT

3PRT.S LISTIT

FORPWR 28PINI E36 57411 05/14/81 16:23:04

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LTCPS

FTM 991M2005/14/81-16:3316.1

SUBROUTINE LTCPS

* LTCP 10

PROCESS LOW TEMPERATURE CPMHS (VIA MHS 1/0)

```

COMMON /CONST/ ATNH,CHFT,PAIM,PAR,PAR,PAR,PAR
COMMON /LOWTH/ MLTSP,SL(10,3),TL(10,3),CPL(10,3),ML(10,3)
COMMON /CONSP/ SL(10,3),ILSP(10)
COMMON /CCC/GRAPH,OUT,IN,END

```

MLTSP=0

CALL NEWPAG

WRITE (JOUT,1010)

1010 FORMAT (1, TYPE, NUMBER OF LOW TEMPERATURE SPECIES TO BE ENTERED)

READ (5,*) MLTSP

LOOP FOR EACH SPECIES

DO 40 I=1,MLTSP

WRITE (JOUT,1012)

1012 FORMAT (1, TYPE SPECIES NAME, IN A12 FORMAT)

READ (JOUT,1014) (SUBLT(I,J),J=1,3)

1014 FORMAT (3A1)

WRITE (JOUT,1020)

1020 FORMAT (1, TYPE NUMBER OF TEMPERATURES FOR THIS SPECIES (1-3))

30 READ (5,*) NT

DO 30 J=1,NT .OR. NT.GT.3) GO TO 30

LOOP FOR EACH TEMPERATURE

DO 50 M=1,NT

WRITE (JOUT,1030)

1030 FORMAT (1, TYPE TL,CPL,ML,SL WHERE)

XSL, TL = TEMPERATURE

XCL, CPL = CONSTANT PRESSURE SPECIFIC HEAT

XSL, ML = ENTALPHY

XSL, SL = ENTROPY

READ (5,*) TL,CPL,ML,SL

ILSP(I)=ILSP(I)+1

CPL(I)=CPL(I)+CPL

ML(I)=ML(I)+ML

SL(I)=SL(I)+SL

CONTINUE

CONTINUE

END SPECIES LOOP

CONTINUE

RETURN

END

END FTM 113 IBANK 182 DRAWN 650 COMMON

AMDSP

MAIN

MAIN

BTM.S MAIN,MAIN

PN 971205718781=1813315.7

1. C MAIN PROGRAM

MAIN0002

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53. X'SICL' .00 .00 X'SICL' .02 .00 .00
54. X'SICL' .03 .00 .00 X'SICL' .04 .00 .00
55. X'SIM' .00 .00 .00 X'SIM' .00 .00 .00
56. X'SIM' .00 .00 .00 X'SI2' .00 .00 .00
57. X'SI20' .00 .00 .00 X'SI2N' .00 .00 .00
58. X'SI3' .00 .00 .00
59. X /
60. DATA YES/YES /
61. DATA INAM/10/
62. DATA JOUT/6/
63. C
64. CALL INI111120/
65. CALL TERM13,1024/
66. CALL CHR512(4)
67. FIRST=.TRUE.
68. IPLOI=0
69. DEFINE FILE 11145,2500,V,IP11/
70. CF=-110
71. DO 300 I=1,26
72. MIN111=0.0
73. F111=0.
74. Y111=0.
75. 300 V111=0.0
76. IP=.FALSE.
77. MP=.TRUE.
78. TV=.FALSE.
79. UV=.FALSE.
80. SV=.FALSE.
81. SU=0.0
82. SP=.FALSE.
83. SMOCK=.FALSE.
84. DETN=.FALSE.
85. MMNG=.FALSE.
86. PS1A=.TRUE.
87. MSOM=.FALSE.
88. IONS=.FALSE.
89. TOCP0C=0
90. FA=.FALSE.
91. OF=.TRUE.
92. ERA110=.FALSE.
93. EPCT=.FALSE.
94. EOL=.TRUE.
95. 010=.FALSE.
96. 101VPE=0
97. DO 320 J=1,10
98. ORCOL111=0.
99. PCTCNV111=0.
100. RECOL111=0.
101. DO 310 J=1,6
102. MCOL111=0.
103. 310 CONTINUE
104. 320 CONTINUE
105. NEAR=.FALSE.
106. 2. CCMI111
107. WFEAC=0
108. NSEPT=0
109.
110.

```

. MAIN022


```

167. GO TO 97
168. C
169. C EMECH INSERT CARDS
170. C 108 CONTINUE
171. CALL NEWPAG
172. WRITE (JOUT,10020)
173. 10020 FORMAT ('-TYPE SPECIES TO INSERT IN A12 FORMAT-')
174. 101 CONTINUE
175. INSERT=INSERT+1
176. READ (5,207) (INSERT(I),I=1,3)
177. IF (INSERT(I).NE.PLANK) GO TO 181
178. INSERT=INSERT+1
179. GO TO 203
180. C
181. C CHECK OMIT CARDS
182. C 205 CONTINUE
183. CALL NEWPAG
184. WRITE (JOUT,10022)
185. 10022 FORMAT ('-TYPE SPECIES TO OMIT FROM JMEMRD DATA, IN A12 FORMAT-')
186. 206 CONTINUE
187. OMIT=OMIT+1
188. READ (5,207) (OMIT(I),I=1,3)
189. 207 FORMAT('JAN')
190. IF (OMIT(I).NE.PLANK) GO TO 206
191. OMIT=OMIT+1
192. 208 CONTINUE
193. NEW=TRUE.
194. REWIND 5
195. GO TO 203
196. C
197. C BEGIN NAMELIST INPT2
198. 210 CALL NEWPAG
199. WRITE (JOUT,10030)
200. 10030 FORMAT ('TYPE YES FOR PRINT INPT2 NAMELIST')
201. READ (5,10032) YES
202. 10032 FORMAT ('N')
203. IF (YES.NE.YES) GO TO 1211
204. C ACCESS THE ORIGINAL NAMELIST FROM PREVIOUS RUN
205. REWIND INAM
206. READ (INAM,INPT2)
207. WRITE (JOUT,INPT2)
208. IF (JOUT.EQ.0) PAUSE
209. CALL NEWPAG
210. GO TO 1212
211. C
212. C RESET ALL PARTS OF NAMELIST
213. 1211 DO 1210 I=1,27
214. 1210 V(I)=0
215. 1211 DO 1210 I=1,27
216. 1210 V(I)=0
217. TP=FALSE.
218. MP=TRUE.
219. TV=FALSE.
220. UV=FALSE.
221. SV=FALSE.
222. PNT=FALSE.
223. SD=0.0

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* MAIN0062

* MAIN0063

* MAIN0065

MAIN

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224. SP=FALSE.
225. SNOCH=FALSE.
226. DEVM=FALSE.
227. MMHC=FALSE.
228. PSIA=TRUE.
229. WSON=FALSE.
230. TONS=FALSE.
231. IDERUG=0.
232. FA=FALSE.
233. OF=TRUE.
234. CRATIO=FALSE.
235. FCT=FALSE.
236. GO TO 1211.
237. 1212 WRITE (JOUT,10034)
238. 10034 FORMAT (I,TYPE YES TO CHANGE NAMELIST*)
239. READ (5,10032) YES
240. IF (YES=NE) YES GO TO 2213
241. 11211 WRITE (JOUT,10036)
242. 10036 FORMAT (I,BEGIN NAMELIST INPUT*)
243. 2211 CONTINUE
244. READ (5,10012)
245. CALL NEWPAG
246. 2213 WRITE (JOUT,10040)
247. 10040 FORMAT (I,TYPE YES FOR PRINT OF COATA NAMELIST*)
248. READ (5,10032) YES
249. IF (YES=NE) YES GO TO 2210
250. REMIND=2444
251. READ (11NAM,COATA)
252. WRITE (JOUT,COATA)
253. IF (JOUT=0) IF TRUE
254. CALL NEWPAG
255. GO TO 2219
256. 2210 OT=FALSE.
257. 10040=0.
258. DO 2230 I=1,10
259. DECIMAL I=0.
260. PCTCHW I=0.
261. ACCURACY I=0.
262. DO 2220 J=1,6
263. DECIMAL J=0.
264. 2220 CONTINUE
265. 2230 CONTINUE
266. 2219 WRITE (JOUT,10052)
267. 10052 FORMAT (I,TYPE YES TO CHANGE COAL DATA NAMELIST*)
268. READ (5,10032) YES
269. IF (YES=NE) YES GO TO 2214
270. 2216 WRITE (JOUT,10044)
271. 10044 FORMAT (I,BEGIN NAMELIST COATA INPUT*)
272. NEW 15,COATA)
273. IF (10044=0) GO TO 2214
274. IF (10044=0) GO TO 2214
275. CALL ENDOFF
276. STORE NAMELIST
277. 2214 REMIND=2444
278. WRITE (11NAM,INPUT)
279. WRITE (11NAM,COATA)
280.

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MAIN

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281.  ENDFILE IMAM
282.  IF (JOUT.EQ.6) PAUSE
283.  GO TO 203
284.  215 CONTINUE
285.  FIRST=.FALSE.
286.  CALL NEWPAG
287.  WRITE (JOUT,10050)
288.  10050 FORMAT (1 TYPE YES FOR PRINT TO ALTERNATE PRINT FILE)
289.  READ (5,10032) VYES
290.  IF (VYES.EQ.VYES) JOUT=31
291.  REWIND IMAM
292.  READ (IMAM,10031)
293.  WRITE (6,10032)
294.  IF (JOUT.EQ.6) PAUSE
295.  CALL NEWPAG
296.  READ (IMAM,COATA)
297.  WRITE (JOUT,10052)
298.  10052 FORMAT (1 TYPE YES TO PRINT COAL DATA NAMELIST)
299.  READ (5,10032) VYES
300.  IF (VYES.EQ.VYES) GO TO 216
301.  WRITE (6,COATA)
302.  IF (JOUT.EQ.6) PAUSE
303.  CALL NEWPAG
304.  216 CONTINUE
305.  WRITE (6,10054)
306.  10054 FORMAT (1 TYPE YES TO SAVE PLOT DATA)
307.  READ (5,10032) VYES
308.  IF (VYES.EQ.VYES) GO TO 210
309.  10056 FORMAT (1 TYPE YES TO PRINT COAL DATA NAMELIST)
310.  READ (5,10032) VYES
311.  IF (VYES.EQ.VYES) GO TO 210
312.  10058 FORMAT (1 TYPE YES TO SAVE PLOT DATA)
313.  IF (JOUT.EQ.6) PAUSE
314.  CALL NEWPAG
315.  10060 FORMAT (1 TYPE YES IF BLANK PLOT TAPE)
316.  READ (5,10032) VYES
317.  IF (VYES.EQ.VYES) GO TO 210
318.  IF (JOUT.EQ.6) PAUSE
319.  READ (11,1) IPLY,MSIPLY
320.  ISPLY=IPLY
321.  IPLY=IPLY+1
322.  210 IFCO=0
323.  IFCO=0
324.  IFCO=0
325.  101=0
326.  DO 2000 I=1,IC
327.  IF (I.EQ.1) IFCO=1
328.  IF (I.EQ.1) IFCO=1
329.  IF (I.EQ.1) IFCO=1
330.  2000 CONTINUE
331.  2002 DO 2004 I=1,IC
332.  IF (I.EQ.1) IFCO=1
333.  IF (I.EQ.1) IFCO=1
334.  2004 CONTINUE
335.  2006 IF (I.EQ.1) IFCO=1
336.  IFCO=0
337.  IFCO=0

```

MAIN

```

338. 177=1
339. 177=1
340. 902 IF (108C.CO.01) GO TO 906
341. 906 IPEB=OCTCNV(IYV)
342. ICDN=OCCOAL(IYV)
343. 906 IF (IUCM1.CO.01) GO TO 920
344. IUCM2=0
345. DO 910 I=1,6
346. IF (IUCOAL1(I,22)) 912,
347. IUCP2=IUCR2+1
348. 910 CONTINUE
349. 912 177=1
350. 914 IUCOCONC=IUCV777
351. 916 BEGIN INAM
352. 918 IYV=IYV+1
353. 918 IYV=OCCOAL(IYV)
354. IF (IYV.CO.01) GO TO 918
355. IF (IYVPT.WC.21) GO TO 918
356. 918 IYV=IYV+1
357. 918 IYV=IYV+1
358. 918 IYV=IYV+1
359. 918 CONTINUE
360. 918 CALL COLCV3(IYV,IYV,IYV)
361. 918 CALL COLCV3(IYV,IYV,IYV)
362. 918 CONTINUE
363. 918 IF (IYV.CO.01) GO TO 1215
364. 918 IF (IYV.CO.01) GO TO 1215
365. 918 IF (IYV.CO.01) GO TO 1215
366. 918 IF (IYV.CO.01) GO TO 1215
367. 918 IF (IYV.CO.01) GO TO 1215
368. 918 IF (IYV.CO.01) GO TO 1215
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371. 918 IF (IYV.CO.01) GO TO 1215
372. 918 IF (IYV.CO.01) GO TO 1215
373. 918 IF (IYV.CO.01) GO TO 1215
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388. 918 IF (IYV.CO.01) GO TO 1215
389. 918 IF (IYV.CO.01) GO TO 1215
390. 918 IF (IYV.CO.01) GO TO 1215
391. 918 IF (IYV.CO.01) GO TO 1215
392. 918 IF (IYV.CO.01) GO TO 1215
393. 918 IF (IYV.CO.01) GO TO 1215
394. 918 IF (IYV.CO.01) GO TO 1215

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452. ENM(J) = 0.
453. IF (IUSE(J).NE.0) GO TO 432
454. ENM(J) = ENM/INS - NC1
455. ENM(J) = ALOG(ENM(J,1))
456. 432 CONTINUE
457. I01 = L+1
458. IF (INC-EO-0-OR-NSCET-EO-0) GO TO 700
459. DO 302 I=1,NSCET
460. DO 301 J=1,NS
461. IF(IUSE(J).EQ.0) GO TO 301
462. DO 299 IST = 1,3
463. 299 IF (SUB(J,IST) .NE. ENSFRT(IST,1)) GO TO 301
464. 301 CONTINUE
465. IUSE(J) = -IUSE(J)
466. GO TO 302
467. 302 CONTINUE
468. 302 CONTINUE
469. 790 IF (.NOT. TP .AND. .NOT. MP .AND. .NOT. SP) GO TO 791
470. CALL TWRMP
471. IF (I07.OR.I0XC.NE.0.OR.IUCR2.NE.0) REPEAT=.TRUE.
472. IF (I07.NE.0) GO TO 916
473. 970 IF (IUCR2.EQ.0) GO TO 980
474. IF (I1X.EQ.IUCR2) GO TO 980
475. I1X=I1X+1
476. GO TO 916
477. 980 IF (I0XC.EQ.0) GO TO 800
478. IF (I1Y.EQ.I0XC) GO TO 800
479. I1Y=I1Y+1
480. I22=I22+1
481. IF (IUCR1.EQ.1) I22=1
482. GO TO 904
483. 791 IF (I07.NE.0) CALL OCTON
484. IF(I07) CALL POCKET
485. IF (I00T.EQ.6) PAUSE
486. IF(SHOCK) CALL SHCK
487. 800 NSERT = 0
488. IF (I1P.EQ.1) GO TO 2
489. NSVPL=NSVPL+1
490. NUM=IPLT-1-ISPLY
491. IS=ISPLY+1
492. WRITE (11,15) IPLNAM,NUM
493. WRITE (11,11) IPLT,NSVPL
494. ISPLY=IPLY
495. IPLT=IPLT+1
496. GO TO 2
497. 3 CONTINUE
498. CALL NEWPAG
499. CALL FINITIO,7001
500. END

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MAIN0153

END FTM 1105 IBANK 1189 DRANK 11272 COMMON

3406,P MATR14

MATRIX

3PTIN,5 MATRIX, MATRIX

FTN 981M2005/214/01-16:33:13.9

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1. SUBROUTINE MATRIX
2. C
3. COMMON/POINTS/MSUM(13),SSUM(13),CPRI(13),DLVTP(13),DLVPT(13)
4. 1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),UM(13),SONVEL(13),TTT(13)
5. 2 ,VLH(13),TOM(13)
6. INCLUDE SPECOP,LIST
7. COMMON /SPECES/EN(150,13),ENL(150),S(1,0),HO(150),DELN(150),
8. SUR(150,3),IUSE(150),SLN(150),TEMP(50,2)
9. X ,COEF(2,7,150),A(25,150)
10. COMMON /MISC/ ENN,SUM,IT,SO,ATOM(13,101),LLMT(25),BO(25),
11. BOPI(25,2),TM,TLOW,TM10,TM16M,PP,CPSUM,OF,(QRAT,
12. MSUBD,AM(2),MP(2),RM(2),VMIM(2),VPLS(2),MP(2),
13. DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECUT(25),
14. ENTM(25),FAZ(25),PI(25),FOI(25),DEMS(25),RMOP,
15. RPM(25),TLN,ORF(26),LNNL,FNSAVE,ENLSAV
16. COMMON /DOUBLE/ G(20,21),X(20)
17. COMMON /INDX/ IDERUS,CONVG,IP,MP,SP,ISV,MOLES,MP,NT,NPT,L,NS,
18. KMAT,IMAT,IOI,NOF,NOM(1),IP,NEWR,IONS,NC,JSOL,JULIO,
19. NREAC,IC,JSI,VOL,SHOCK,IT,NPZ,CALCH,IOSAVE,LSAVE
20. DOUBLE PRECISION G,X
21. LOGICAL CONVG,MP,SP,IP,VOL
22. C
23. IQ2 = IQ1 + 1
24. IQ3 = IQ2 + 1
25. SP,IP,NOF,CONVG,AND,IP) KMAT = IQ2
26. C CLEAR MATRIX STORAGES TO ZERO
27. DO 211 I=1,NPT
28. DO 211 J=1,NPT
29. DO 211 K=1,NMAT
30. SSS = 0.
31. RSUMPTT = 0.
32. C BEGIN SET UP OF ITERATION MATRIX
33. NR = L
34. DO 65 J=1,NS
35. IF IUSE(J),LT,01 GO TO 65
36. IF IUSE(J),GT,01 GO TO 70
37. F = (MOI(J)-SI(J)+ENL(NJ)+TM)*ENI(J,NPT)
38. SS = MOI(J)*ENI(J,NPT) - F
39. TERM = -MOI(J)*ENI(J,NPT)
40. IF (IMAT.EQ.102) TERM = F
41. DO 55 I = 1, L
42. C CALCULATE THE ELEMENTS RI(I,K)
43. IF (AT(I,J).EQ.0.) GO TO 55
44. DO 15 K=1,L
45. G(I,K) = G(I,K) + A(I,J)*AT(I,J)*ENI(J,NPT)
46. G(I,101) = G(I,101) + A(I,J)*ENI(J,NPT)
47. G(I,102) = G(I,102) + A(I,J)*TERM
48. IF (CONVG.OR,IP) GO TO 55
49. G(I,103) = G(I,103) + A(I,J)*F
50. IF (FPT)-G(I,102,11) = G(I,102,11) + A(I,J)*SS
51. SS CONTINUE
52. IF (IMAT.EQ.102) GO TO 64

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MATRIX

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1 61. IF (CONV, OR, MP) GO TO 50
1 54. G1102,101 = G1102,101 * SS
1 55. G1102,102 = G1102,102 * M01J055
1 56. G1102,103 = G1102,103 * S1J - ENLN(J1-TM10F
1 57. GO TO 67
1 58. 59 G1102,102 = G1102,102 * M01J052 * EN(J,NPT)
1 59. IF (CONV) GO TO 64
1 60. G1102,103 = G1102,103 * M01J05F
1 61. 62 G1101,103 = G1101,103 * F
1 62. 64 G1101,102 = G1101,102 * F * M1
1 63. GO TO 65
1 64. C CONDENSED SPECIES
1 65. 70 KK = KK + 1
1 66. DO 75 I = 1,L
1 67. G11,KKI = M11,J1
2 68. 75 G11,MMAT = G11,MMAT - A11,J1 * EN(J,NPT)
1 69. G11,102 = M11,J1
1 70. G11,MMAT = M01J1 - S1J
1 71. MSUM(NPT) = MSUM(NPT) + M01J1 * EN(J,NPT)
1 72. IF (.NOT. SP) GO TO 65
1 73. SSS = SSS + S1J * EN(J,NPT)
1 74. G1102,MM = S1J
1 75. 65 CONTINUE
1 76. SSS = SSS + G1102,101
1 77. MSUM(NPT) = MSUM(NPT) + G1101,102
1 78. G1101,101 = SUMN - ENN
1 79. C REFLECT SYMMETRIC PORTIONS OF THE MATRIX
1 80. K = 101
1 81. IF (MP) OR (CONV) K = 102
1 82. DO 102 I = 1,M
1 83. DO 102 J = 1,M
1 84. 102 84.11 = G11,11
2 85. C COMPLETE THE RIGHT HAND SIDF
1 86. IF (CONV) GO TO 175
1 87. DO 195 I = 1,L
1 88. X11 = M11 - G11,101
1 89. 195 G11,MMAT = G11,MMAT + X11 * ENN - SUMN
1 90. C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
1 91. IF (MP) .EQ. 102 GO TO 185
1 92. IF (SP) ENERGY = SD * ENN - SUMN - SSS
1 93. IF (MP) ENERGY = MSUB0 / T1 - MSUM(NPT)
1 94. G1102,101 = G1102,101 * ENERGY
1 95. 175 G1102,102 = G1102,102 * CP * SUM
1 96. 185 IF (.NOT. VOL OR (CONV)) RETURN
1 97. C CONDENSED SPECIES
1 98. K = 101 - 1
1 99. IF (MMAT.EQ.102) GO TO 270
1 100. DO 220 I = 1,M
1 101. 220 101.11 = G1102,11 * G1101,11
1 102. G11,101 = G11,102 - G11,101
1 103. 720 G11,102 = G11,103
1 104. G1101,101 = G1102,102 - G1101,102 * G1101,101
1 105. G1101,102 = G1102,103 - G1101,103
1 106. IF (MP) G1101,102 = G1101,102 * F * M1
1 107. GO TO 260
1 108. 230 DO 240 I = 1,M
1 109. 240

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MATRIX

110. 280 GIL1011 - GIL1021

111. 280 KMAT = IMAT

112. IMAT = IMAT-1

113. RETURN

114. END

. MATX0090

END PTH 200 THINK 43 DBANK 11345 COMMON

3M06,P NEWOF

MEMOF

```

8FTN.5 MEMOF, MEMOF
FTN 9R1W2005/14/781-16:3311,1
SUBROUTINE MEMOF
1.
2. C SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES
3. C
4. C
5. COMMON /CONSTS/ ATN,GMET,PAIM,RBAR,RPR,RVR /CONSTS/
6. COMMON /MOLCOM/ END,GAS,IE,IZERO,LANH,MOL,OF,ZERO /MOLCOM/
7. COMMON /MISC/ ENN,SUMN,TI,SO,ATOM(3,101),LLMT(25),BO(25), /MISC/
8. BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,
9. MSUBQ,M(12),MPP(12),RM(12),VMIN(12),VPLS(2),MPL(2),
10. DATA(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECMT(25),
11. CWM(125),FRT(25),FRTCHP(25),FRT(25),DENST(25),RHOP,
12. RMW(25),TLN,OXF(26),ENHL,ENSAVE,ENLSAV
13. COMMON /INDX/ IGERUG,COMVG,TP,HP,SP,ISV,MOLES,IMP,IMPNT,INLMINS, /INDX/
14. KMAT,IMAT,IQI,MOF,NOMIT,IF,NEUR,IONS,INC,JSOL,JLIO, /INDX/
15. NREAC,IC,JSI,VOL,SMOCK,IT,MFZ,CALCM,ISAVE,LSAVE /INDX/
16. C
17. COMMON /CCCT/ GRPM,JOUI,TDEWIND
18. COMMON /CFUEL/CF,MHVA,CCR,PER,CCR
19. C
20. LOGICAL CALCM,VOL
21. DATA FUD/MH,CF,FHM/5MH,C/FCAL/4HAL/G/
22. C CALCULATE NEW VALUES OF RD AND MSUBQ FOR NEW OF RATIO
23. MBLIE,JOUI,JOUI OF
24. 730 FORMAT(6HOOF = ,F10.6)
25. 1E OF 1.01,302,
26. 1E OF 1.01,302,
27. WRITE (JOUT,732) CF,MCR,PER,CCR
28. 732 FORMAT (21X,'FRTOTZER/COAL=',F8.4,5X,'WATER/COAL=',F8.4,
29. X 5X,'CARBON CONVERSION=',F8.4,5X,'RECYCLE CARBON/COAL=',F8.4)
30. 302 CONTINUE
31. SUM = OF + 1.
32. V2 = TOF*VMINT(1)+VMINT(2)/SUM
33. V1 = (OF*VPLS(1)+VPLS(2))/SUM
34. IF (V2 .LT. 0.0) EORAT = ABS(V1/V2)
35. IF (RM(1)+GL,0.0 .AND. RM(2)-GL,0.0) GO TO 744
36. RHOP = RM(2)
37. IF (RHOP .LE. 0.0) RHOP = RM(1)
38. GO TO 745
39. 744 RHOP = (OF+1,FORM(1)+RM(2)/RM(1))+ OF *RM(2)
40. 745 DO 747 J = 1,N
41. 747 BQ(1) = (BOP(1,2) + BOP(1,1)*OF)/SUM
42. IF (.NOT. CALCM) GO TO 750
43. CALL RECALC
44. CALCM = .FALSE.
45. IF (OF .GT. 0.0) HPP(1) = SUM*HPP(1)/OF
46. HPP(2) = SUM*HPP(2)
47. GO TO 750
48. 750 MSUBQ = (HPP(2) + HPP(1)*CF)/(IRAP+OSUP)
49. 750 IC = C
50. JSOL = 0
51. JLIO = 0
52. MS = 0
53. 750 MSUBQ = MSUBQ
54. 750 MSUBQ = MSUBQ
55. 770 FORMAT (10D,17X,4HFUEL,13X,7HOXIDANT,12X,7HMIXTURE, /)

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NEUOF

MAIN012

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56. 780 FORMAT (1M,3A,3E18.8/1
57.  FF = FWH
58.  IF (VOL)FF = FUU
59.  WRITE(JOUT,780) FF,FCAL ,HPP(2),HPP(1),MS
60.  WRITE(JOUT,781)
61.  785 FORMAT (12M,10A,10E18.8/1
62.  WRITE(JOUT,780) ILLMT(I),LANH,80P(J,2),80P(J,1),80(J), J = 1,NLM)
63.  RETURN
64.  END
    
```

END FTN 132 IBANK 150 DRANK 1016 COMMON

ENDG,P OUT1

OUT1

BEIN,S OUT1,OUT1

FTN 991M2005/14/01-16:33124,1

1. SUBROUTINE OUT1

• OUTP0001

• /MOLCOM/

• /MISC/

• /MISC/

• /MISC/

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• OUTP0002

• OUT1 5AD

• OUT1 610

OUT1

DATE 051401

PAGE

2

64. 4015-1401-231-COF, WCR, PER, CCR
57. 22 FORMAT 121X, OXIDIZER/COAL=, F8.4, 5X, WATER/COAL=, F8.4,
58. 5X, CARBON CONVERSION=, F8.4, 5X, RECYCLE CARBON/COAL=, F8.4,
59. 6X RETURN
60. END

. OUTP0137

END FIN 125 IRANK 241 DRANK 1589 COMMON

ENDG.P

OUT2

111355391-18/91/5002M1B4 N13

COMMON/POINTS/MSUM(I3),SSUM(I3),CPRI(I3),OLVTP(I3),OLVPT(I3)

.yLm0139.T01N(13)

KWAT, IMAI, IOI, NOF, NOMIT, I, P, NEWB, IONS, NC, JSOL, JLIQ, . /YNDX/

COMMON /PERF, PCF(26),VMOC(13),SPIN(13),VACI(13),SUGAR(13),

COMMON /DPLOT/PLOT(45,13),YPLT,YPLT1,NSIPLT

ONE, TWO, ZERO, FIVE, FIVE, FIVE

DIMENSION F6(2), FY(2), FW(2), FX(2), FAP(2), FCP(2),

[illegible][illegible]

000-000-000-000-000

[illegible]

DIMENSION FPP121, FTR121, FMW121, FSS121

1 1936.00 4M31.0612.013-1.0617.0041 1111

DATA IFSSII, I=1, 21/5 RTU/ , (LB-A) /

1130 - 002
1130 - 002
1130 - 002

(LAWYER) JAMES L. BROWN

FLAG=0

FLA 62:1

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F (IFLAG.EQ.0) V(I)=A1MNOPP(I)

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ON VINUE

[illegible]

14M'1=1 95 0

REPORT—

2000

OUT2

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56. DO 60 I=1,NPT
57. 60 V(I)=V(I,I)
58. IF (IFLAG.EQ.0) GO TO 74
59. DO 72 J=1,NPT
60. 72 V(J)=V(I,I)-273.15*0.032
61. 74 IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FV,F8,(V(I,J),J=1,NPT)
62. IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FV,F8,(V(I,J),J=1,NPT)
63. DO 73 I=1,NPT
64. 73 PLOT(2,I)=V(I)
65. C ENTHALPY
66. DO 75 I=1,NPT
67. 75 I=BAROMSUM(I)
68. IF (IFLAG.EQ.1) V(I)=V(I)*1.0
69. 75 CONTINUE
70. IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FM,F8,(V(I,J),J=1,NPT)
71. IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FM,F8,(V(I,J),J=1,NPT)
72. DO 76 I=1,NPT
73. 76 PLOT(2,I)=V(I)
74. C ENTROPY
75. FMT(4)=FOUR
76. DO 78 I=1,NPT
77. 78 V(I)=BAROSSUM(I)
78. IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FS,F8,(V(I,J),J=1,NPT)
79. IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FS,F8,(V(I,J),J=1,NPT)
80. C DENSITY
81. DO 80 I=1,NPT
82. 80 V(I)=V(I)*1.0
83. IF (IFLAG.EQ.1) V(I)=V(I)*1.0206/35.31
84. 80 PLOT(3,I)=V(I)
85. IF (IFLAG.EQ.0) WRITE (JOUT,FMT) FV,F8,(V(I,J),J=1,NPT)
86. 1 FORMAT (1X,10DENSITY G/CC ,1P13E9.3)
87. IF (IFLAG.EQ.1) WRITE (JOUT,FMT) FV,F8,(V(I,J),J=1,NPT)
88. 2 FORMAT (1X,10DENSITY L/1000 ,1P13E9.3)
89. WRITE(JOUT,FO)
90. PD FORMAT ' 1M '
91. C MOLECULAR WEIGHT
92. WRITE (JOUT,FMT) FM,F8,(V(I,J),J=1,NPT)
93. C TOLV/PLV
94. IF (EQL) WRITE (JOUT,FMT) FT,F8,(V(I,J),J=1,NPT)
95. C TOLV/DELTA
96. IF (EQL) WRITE (JOUT,FMT) FV,F8,(V(I,J),J=1,NPT)
97. C MEAT CAPACITY
98. DO 95 I=1,NPT
99. 95 V(I)=BAROSSUM(I)
100. WRITE (JOUT,FMT) FCP,F8,(V(I,J),J=1,NPT)
101. C GAMMA(S)
102. WRITE (JOUT,FMT) FCP,F8,(V(I,J),J=1,NPT)
103. C SONIC VELOCITY
104. PLOT(4,I)=FO
105. DO 95 I=1,NPT
106. 95 SONVEL(I)=SQRT(PBAROSSUM(I)*V(I,I)/V(I,I))
107. WRITE (JOUT,FMT) FSV,FVEL,(SONVEL(I),J=1,NPT)
108. IF (JOUT.EQ.6) FALSE
109. CALL NEWPAG
110. RETURN
111. END

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OUT2

END FOR 285 18AVE 882 DRANK 10A1 COMON

END P OUT3

DATE 051003

PAGE 3

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OUT

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1 53. CMW111=MM111*SUM
1 54. S02 CONTINUE
55. WRITE (JOUT,520) (CMW111,I=1,NPT)
56. FORMAT 1X,10F10.5
57. C LOCATE DRY ELEMENTS
58. DO 510 I=1,15
59. DO 508 J=1,NS
60. DO 506 K=1,3
61. IF (JDK11(K).NE.1508(J,K)) GO TO 508
62. S06 CONTINUE
63. INDX11=J
64. DO 507 L=1,NPT
65. S07 PLOT(23,1)=CMW111
66. GO TO 510
67. S08 CONTINUE
68. INDX11=0
69. DO 509 L=1,NPT
70. S09 PLOT(23,1)=L
71. S10 CONTINUE
72. C LOOK FOR ANY SOLIDS OR LIQUIDS NOT IN TABLE
73. DO 1502 I=1,NPT
74. PLOT(39,1)=0
75. DO 1510 J=1,NS
76. IF (IUSE1(J).LE.0) GO TO 1510
77. C EXCLUDE CASH AND ICASH
78. IF (INDX11).EQ.0 GO TO 1510
79. IF (INDX12).EQ.0 GO TO 1510
80. S106 PLOT(39,1)=PLOT(39,1)+CMW111
81. S150 CONTINUE
82. DO 516 I=1,NPT
83. S09=0
84. DO 514 J=1,6
85. IJ=INDX1(J)
86. IF (IJ.EQ.0) GO TO 514
87. S08=SUM+EM1(J,I)
88. S19 CONTINUE
89. XOP11=SUM/YO1N11
90. S16 CONTINUE
91. WRITE (JOUT,520) (XOP11,I=1,NPT)
92. FORMAT 1X,10F10.5
93. DO 522 I=1,NPT
94. YOPS11=(305.2*XOP11)/(CMW111)*(1./CF1*(1.-OF1))
95. S22 CONTINUE
96. WRITE (JOUT,520) (YOPS11,I=1,NPT)
97. FORMAT 1X,10F10.5
98. L1=INDX11
99. L3=INDX13
100. L4=INDX14
101. DO 530 I=1,NPT
102. SUM=C
103. IF (L4.NE.0) SUM=SUM+319.24*EM1(L4,I)/TOTN11
104. IF (L3.NE.0) SUM=SUM+316.06*EM1(L3,I)/TOTN11
105. IF (L1.NE.0) SUM=SUM+99.4*EM1(L1,I)/TOTN11
106. HHVS11=SUM/XOP11
107. S10 CONTINUE
108. WRITE (JOUT,520) (HHVS11,I=1,NPT)
109.

```

OUT4

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110. 532 FORMAT(1X,'MMV SAT 0/SCF',1X,13F9.2)
111. DO 530 I=1,NPT
112.  CEF11=MMVS(I)*PPS(I)*MMV
113.  VLP(I)=770.5*DS(I)/305.2
114.  MMVD(I)=385.2/379.51*MMVS(I)
115.  IF (LONE.O) LMVS(I)=MMVS(I)-1059.9*18./385.2*(EM(LN,I)/TOTN(I))
116.  I=7*NP1
117.  LMVD(I)=LMVS(I)+385.2/379.5
118.  DOL(I)=10000.*11.25*MMV/10000.*OF/CF*(MMVS(I)*VDPST(I))
119.  530 CONTINUE
120.  WRITE (JOUT,542) (CEF11,I=1,NPT)
121.  542 FORMAT(1X,'EFFICIENCY',1X,13F9.5)
122.  WRITE (JOUT,544) VDPST(I)=1,NPT
123.  544 FORMAT(1X,'V DRY SCF/LB',1X,13F9.5)
124.  WRITE (JOUT,546) (MMVD(I),I=1,NPT)
125.  546 FORMAT(1X,'MMV DRY 0/SCF',1X,13F9.2)
126.  WRITE (JOUT,548) (LMVS(I),I=1,NPT)
127.  548 FORMAT(1X,'LMV SAT 0/SCF',1X,13F9.2)
128.  WRITE (JOUT,550) (LMVD(I),I=1,NPT)
129.  550 FORMAT(1X,'LMV DRY 0/SCF',1X,13F9.2)
130.  WRITE (JOUT,552) (DOL(I),I=1,NPT)
131.  552 FORMAT(1X,'S PER MMBTU',1X,13F9.2)
132.  560 CONTINUE
133.  RETURN
134.  END

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. OUTP0137

A-1 END FTM 365 IPANN 506 08ANN 11061 COMPCN

AMOG,P PLOT8007

0FRT,5 PLOT8007
FURPUR 28R1M1 E36 574711 05/10/81 16:33:51

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PLOTB00T

SE4JGMB JN208e TPF S1D1.PLOTB00T

- 1 ACAT, P 11, F/2/POS/2
- 2 BASG, A 11.
- 3 BASG, T PLOT, U9S.
- 4 SCOPY, G PLOT, 11.

ANDG.P PLOTON

GPRT.S PLOTON

FURPUM 200JHJ E36 S7AT11 05/10/81 16133102

PL010N

DATE 051481 PAGE 1

SEVICM01208010F51010P010N
1 00SG,1 PLOT,U9S,0

0M0G.P PLOTSAVE

0PRT,5 PLOTSAVE
PUMPUR 2001M1 E36 S70111 05/14/81 16:33:03

PLOTSAVE

SEICN81N2001PFA101-PLOTSAVE

- 1 OPENING PLOT.
- 2 COPY-ON 11-PLOT.
- 3 FREE PLOT.

8400:P FROM

PROG

POP.LMF_PROG.PROG
PCP12P1 R72-16 05/14/81 16:33:44 (2.0) RT
PF0001 SPECIM PROC
0002 COMMON /SPECIES/EN(150),S(150),H(150),DEL(150),
0003 X SUR(150,3),IUS(150),SLN(150),TEMP(50,2)
0004 X COEF(2,2,150),A(25,150)
0005 END

END POP ERRORS : NONE

AM06.P REACT


```

56. IC=1
57. C READ REACTANTS
58. REMIND IO
59. 6 READ (IO) NREAC,CF
60. 10 IF (IC.EQ.0) GO TO 20
61. IF (CF-1.C) -18.
62. REACT=0
63. READ (N) NUHMY,CF,MHVV,MCR,PER,CCR
64. 14 IF INDEAC.EQ.0) GO TO 200
65. 2C CONTINUE
66. MOLEZIM
67. IF (IOI.EQ.1) GO TO 22
68. READ (IO) NAME(1),ANUMIN(1),FAZ(M),
69. X NAME(1),ANUMIN(1),FAZ(M),
70. X QTEMPIN),FOXIN),DENSI(M)
71. 22 ENTHIN)=ENTHIN)-HOMADOPHIN)
72. NAST=10LANK
73. IF (NAMEIN(6).EQ.1200.AND.107.EQ.0) NAST=1AST
74. NAST=1JOUT,301,NAMEIN(1),ANUMIN(1),J=1,51,PECMTIN(1),MOLE,
75. X ENTHIN),NAST,FAZ(M),QTEMPIN),FOXIN),DENSI(M)
76. 30 FORMAT (1H,12,2H,5142,5H,2H),F10.6,2H,A1,F12.4,A1,3H,A1,F12.3,
77. X 3H,A1,F12.5,1X)
78. IF (L.EQ.0) GO TO 20
79. IF (MOLE.EQ.0) MOI MOLES = .TRUE.
80. IF OXIDANT, N=1, IF FUEL, N=2.
81. IF (FOXIN).EQ.700) FOXIN)=OX
82. IF (PECMTIN).LE. 0.0) PECMTIN) = 1.0
83. N=1
84. IF (FOXIN).EQ.0X) GO TO 37
85. N=2
86. MFUEL = MFUEL+1
87. 37 GO TO 30-37-25
88. 38 DATA(J) = 0.0
89. R=0.
90. DO 100 JJ=1,6
91. IF (ARURIN,JJ).LE. 0.0) GO TO 101
92. IF (NAMEIN,JJ).EQ. 200) NAMEIN,JJ) = OX
93. DO 81 JJ=1,25
94. I=J
95. IF (LLMT(J).EQ.0) GO TO 85
96. 81 IF (NAMEIN,JJ).EQ. LLMT(J)) GO TO 86
97. L=1
98. LLMT(J)=NAMEIN(JJ)
99. 86 GO TO 81-101
100. 88 IF (ATOM(J).EQ. ANAMEIN,JJ)) GO TO '0
101. L=0
102. GO TO 20
103. 50 RM = RM + ANUMIN,JJ)*ATNM(2,1)
104. 104-101-101-101
105. 100 DATA(J) = ANUMIN,JJ)
106. 101 PCMT=PECMTIN)
107. IF (MOLES) PCMT=PCMTORM
108. WPKIN=MPIN) * PCMT
109. IF (ICT.EQ.1.AND.1CTYPE.EQ.1) NAMEIN,63)=
110. IF (NAMEIN,61.NE.1200) HPPIN)=HPPIN)+ENTHIN)*PCMT/RM
111. AMKIN=MPIN)*PCMT/EP
112. DO 11C J=1,L

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REACT

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1 113. 110 BOP(1,1) = DATA(1,1) + BOP(1,1)
114. IF (DENSI) .GT. 0.01 DM(1) = DM(1) * PCUT/DENSI
115. DM(1) = DM
116. N = N+1
117. IF (M.EQ.2) GO TO 200
118. IF (10.EQ.N) AND (N-1.EQ.MREAC) GO TO 207
119. IF (10.EQ.M) AND (N-1.EQ.MREACT) GO TO 200
120. GO TO 20
121. 200 MREACT=N-1
122. IF (10.EQ.N) GO TO 204
123. TO=MB
124. REFINC TO
125. REFINC MREACT(1,1) + MREACT(1,1)
126. IF (MREACT(1,1) GO TO 204
127. DO 202 I=1,4
128. READ (10) MUMMY
129. 202 CONTINUE
130. GO TO 4
131. 204 MREACT=N
132. IF (10.EQ.1) GO TO 207
133. IF (10.EQ.0) GO TO 206
134. IQ=0
135. GO TO 207
136. 206 IQ=1
137. 207 IF (MUEL(1,1) GO TO 210
138. C 100 PERCENT OXIDANT, CALL REACTANTS FUEL
139. DO 205 N=1,MREACT
140. FOR(N) = 1,M
141. DM(1) = DM(1)
142. DM(1) = DM(1)
143. MP(1) = MP(1)
144. MP(1) = MP(1)
145. MPP(1) = MPP(1)
146. MP(1) = MP(1)
147. AP(1) = 0.
148. DO 208 J=1,L
149. 208 BOP(1,2) = BOP(1,1)
150. 210 IF (1.EQ.0) GO TO 214
151. WRITE (10) (1,2)
152. 212 FORMAT 'YOU: (1,2)'
153. 214 WRITE (10) (1,2)
154. 215 FORMAT ' (1,2)'
155. WRITE (10) (1,2)
156. 329 FORMAT (1,2), (1,2), (1,2), (1,2) ENTHALPY TO BE CALCULATED
157. IF (10.EQ.6) PAUSE
158. CALL KEM(1,2)
159. DO 220 K=1,2
160. IF (MPP(1) .LE. 0.0) GO TO 220
161. MPP(1) = MPP(1) / MPP(1)
162. MP(1) = MP(1) / MP(1)
163. IF (DM(1) .GT. 0.0) DM(1) = DM(1) / DM(1)
164. DO 216 J=1,L
165. BOP(1,1) = BOP(1,1) / DM(1)
166. IF (1,1) .LT. 0.0 DM(1) = DM(1) * DM(1)
167. 215- IF (1,1) .GT. 0.0) DM(1) = DM(1) * DM(1)
168. IF (MOLES) GO TO 220
169. DO 218 N=1,MREACT

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REACT

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2 170. IF (EQ(LN).EQ.OX.AND.N.EQ.2).OR.(EQ(XI).NE.OX.AND.N.EQ.1) GO TO 218
2 171. PECUTIM = PECUTIM/NP(X)
2 172. 218 CONTINUE
1 173. 220 CONTINUE
174. NEW = .TRUE.
175. C ARE ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEW = .FALSE. • 4/23/70
176. IF IL.NE.NLS.CF.NOMTY.NE.OF GO TO 228
177. DO 224 I=1,NLS
178. DO 222 J=1,L
179. IF (LLM(I).NE.LLMTS(I)) GO TO 222
2 180. SROP(I,1) = SROP(J,1)
2 181. SROP(I,2) = SROP(J,2)
2 182. GO TO 224
2 183. 222 CONTINUE
1 184. GO TO 226
2 185. 224 CONTINUE
186. NEW = .FALSE.
187. DO 225 I=1,L
188. LLM(I) = LLMTS(I)
189. SROP(I,1) = SROP(I,1)
190. 225 SROP(I,2) = SROP(I,2)
191. GO TO 224
192. NLS = L
193. NEWIND =
194. DO 228 I=1,L
195. SROP(I,1) = SROP(I,1)
196. SROP(I,2) = SROP(I,2)
197. 228 LLM(I) = LLMTS(I)
198. IF (LLM(I).NE.LLMTS(I).OR.SROP(I,1).NE.SROP(I,1).OR.SROP(I,2).NE.SROP(I,2)) GO TO 230
200. RM(I) = 0.
201. RM(I) = 0.
202. RETURN
203. 230 CONTINUE
204. RETURN
205. END

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END FTV 695 INANK 305 DBANK 1089 COMMON

ENDG.P ANTOUT


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941 C LOOP FOR EACH OF
57. 321 IT = 1
58. 10F = 10F * 1
59. OF = OF/10F
60. CALL NEWOF
61. IF (111) .LE. 0.01 GO TO 322
62. IT = IT+1
63. C LOOP FOR CHANGED PRESSURES
64. 322 DO 99P IP = 1,NP
65. ITNUM = 0
66. AREA = .FALSE.
67. IF (111) .LE. 0.01 MP = .1PUC
68. 3F = 1.0F - 0.5F * IP
69. SP = .FALSE.
70. FOR = .TRUE.
71. 1SUB = 1
72. 1SUP = 1
73. 1P = 1
74. 1P = 1
75. C LOOP FOR PRESSURE RATIOS
76. 331 IF (EQ1) GO TO 332
77. CALL FROZEN
78. GO TO 332
79. 332 CALL COLUPM
80. 1F = 0.1F - 0.01F
81. 1332 IF (111) .GT. 0.01 GO TO 313
82. 1F = 1F + 0.01F
83. 1333 IF (111) .GT. 0.01 RETURN
84. 1334 IF (111) .GT. 0.01 GO TO 313
85. 1335 IF (111) .GT. 0.01 GO TO 313
86. 1336 IF (111) .GT. 0.01 GO TO 313
87. 1337 IF (111) .GT. 0.01 GO TO 313
88. 1338 IF (111) .GT. 0.01 GO TO 313
89. 1339 IF (111) .GT. 0.01 GO TO 313
90. 1340 IF (111) .GT. 0.01 GO TO 313
91. 1341 IF (111) .GT. 0.01 GO TO 313
92. 1342 IF (111) .GT. 0.01 GO TO 313
93. 1343 IF (111) .GT. 0.01 GO TO 313
94. 1344 IF (111) .GT. 0.01 GO TO 313
95. 1345 IF (111) .GT. 0.01 GO TO 313
96. 1346 IF (111) .GT. 0.01 GO TO 313
97. 1347 IF (111) .GT. 0.01 GO TO 313
98. 1348 IF (111) .GT. 0.01 GO TO 313
99. 1349 IF (111) .GT. 0.01 GO TO 313
100. 1350 IF (111) .GT. 0.01 GO TO 313
101. 1351 IF (111) .GT. 0.01 GO TO 313
102. 1352 IF (111) .GT. 0.01 GO TO 313
103. 1353 IF (111) .GT. 0.01 GO TO 313
104. 1354 IF (111) .GT. 0.01 GO TO 313
105. 1355 IF (111) .GT. 0.01 GO TO 313
106. 1356 IF (111) .GT. 0.01 GO TO 313
107. 1357 IF (111) .GT. 0.01 GO TO 313
108. 1358 IF (111) .GT. 0.01 GO TO 313
109. 1359 IF (111) .GT. 0.01 GO TO 313
110. 1360 IF (111) .GT. 0.01 GO TO 313
111. 1361 IF (111) .GT. 0.01 GO TO 313
112. 1362 IF (111) .GT. 0.01 GO TO 313

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POCKET

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113. IF I,SOL -NE. 01 GO TO 925
114. IF I,TMELT -LE. 0.01 GO TO 192
115. DLT = ALOGITMFLT/TTI
116. PP = PP*EXP(DLT*CPRI(2)/(ENNO*DLVTPI(2)))
117. APP(2) = P(PPI)/PP
118. TMI = .TRUE.
119. GO TO 331
120. 925 TMELT = TT
121. 192 APP(2) = APP(1)/11.0 * IUSG = ASQI7(ENNO*ICAMMS(2) * I.0)*DBRRTT(1)
122. PP = P(PPI)/APP(2)
123. ITROT = ITROT-1
124. JELEQ(1) WRITE(JOUT,194) APP(2)
125. 194 FORMAT(7M PC/PF=F9.6)
126. GO TO 331
127. 899 AMT = ENNO*TT/(PP*USQ**5)
128. PCPLT = ALOGIAPP(2)
129. 900 ISV = 0
130. IF 111 -LE. 0.01 GO TO 860
131. AEATIMPT) = ENNO*TT/(PP*USQ**5.5*AMT)
132. IF IAREA) GO TO 800
133. IF IIPP.LI.MPI GO TO 859
134. IF IINSUR.NSUP).EQ.0) GO TO 860
135. AREA = .TRUE.
136. C PCP ESTIMATES FOR AREA PATIOS
137. 800 IF ITNUM.NE.01 GO TO 810
138. DLNP = 1
139. ITNUM = 1
140. ARATIO = SUBAR(IISUB)
141. IF IINSUB.LE.01 ARATIO=SUBAR(IISUP)
142. ELN = ALOGIARATIO)
143. IF IINSUB.LE.01 GO TO 200
144. APPL = PCPLT/(ISUPAR(IISUB)*110*507*ELN**2.9*950)ELN)
145. IF IARATIO.LT.1.091 APPL=.99APPL
146. GO TO 859
147. 799 IF IISUPAR(IISUB).LT.2.1 GO TO 805
148. IF IISUP.GT.1.AND.SUPAR(IISUP-1).GE.2.1 GO TO 802
149. APPL = GAMMAS(2)*ELN*1.4
150. GO TO 859
151. 805 APPL = SQRT(ELN*11.535*Y.294*ELN))PCPLT
152. GO TO 859
153. PIC IF IIDEBUG .LE. 0 .OR. NPT .LT. IDERUG) GO TO 809
154. WRITE(JOUT,181)ITNUM,ARATIO,AEATIMPT),APP(IMP),DLNP
155. 1811 FORAT(6HOITER=12.5X,15HASSIGNED AE/AT=F13.8,5X,6HEE/ATE,F15.8,
156. 15X,5APC/P=F15.8,5X,11HDELTA LN P=F15.P)
157. 809 TOL = 1.0E-5
158. IF IARATIO.GE. 10.0) TOL = 4.0E-5
159. IF IABE(AEATIMPT) - ARATIO)/ARATIO .LE. 10) GO TO 830
160. IF IABS(DLNP) .LT. 4.0E-6) GO TO 830
161. AEATL = ALOGI(AEATIMPT))
162. ITNUM = ITNUM + 1
163. IF IITNUM .GT. 25) GO TO 820
164. ASQ = RR*GAMMAS(IMP)*ENNO*TT
165. CLNPE = GAMMAS(IMP)*USQ/IUSQ-ASQ)
166. 802 DLNP = DLNPE*(LN-DLNP)*AEATL
167. APPL = APPL * DLNP
168. IF IITNUM.EQ.1) GO TO 859
169. APP(IMP) = EXP(APPL)

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1 170. PP = P(IPI)/APP(IPI)
1 171. GO TO 331
1 172. 820 WRITE(JOUT,821) APATIO
1 173. 821 FORMAT(10X,COMPOCKET DID NOT CONVERGE FOR AREA RATIO =,F11.6/)
1 174. P30 ITAUM = 0
1 175. ACALISELL = AREA10
1 176. IF (MSUB.LT.0) GO TO 834
1 177. ISUB = ISUB+1
1 178. IF (ISUB.LE.MSUB) GO TO 800
1 179. ISUB = 1
1 180. MSUB = -MSUB
1 181. IF (ISUB.LE.MSUB) GO TO 800
1 182. GO TO 835
1 183. 834 ISUB = ISUB+1
1 184. IF (ISUB.LE.MSUB) GO TO 800
1 185. ISUB = 1
1 186. 835 AREA = .FALSE.
1 187. GO TO 860
1 188. 839 ISV = NPI
1 189. IF (NPI.NE.131) GO TO 870
1 190. 860 CALL RNTOUT (IGAM)
1 191. IF (IT.LE.0.0) ISV = 0
1 192. IF (.NOT. EOL.AND. IT.LE.0.0) WRITE(JOUT,862)
1 193. 862 FORMAT(17X,125H.CALCULATIONS WERE STOPPED IN ROCKET BECAUSE NEXT
1 194. 1POINT IS MORE THAN 50 DEGREES BELOW TEMPERATURE RANGE OF A CONDENS
1 195. 2ED SPECIES)
1 196. IF (ISV.EQ.0) GO TO 990
1 197. 865 P8256(19M) = 865
1 200. NPI = 2
1 201. 870 NPI = NPI+1
1 202. IF (.NOT.EOL) GO TO 880
1 203. IF (ISV.EQ.1) ISV = -1
1 204. CALL SAVE
1 205. 880 IPI = IPI+1
1 206. IF (NPI.EQ.2) GO TO 331
1 207. IF (.NOT. EOL) IF (NPI) PCPT(IPI)-21
1 208. IF (AREA) APP(IPI)=EXP(1/APPL)
1 209. PP = P(IPI)/APP(IPI)
1 210. GO TO 331
1 211. 990 IF (TOPBUG.LT.0) IDEBUG=IDEBUG+13
1 212. IF (MSUB.LT.0) MSUB=-MSUB
1 213. IF (.NOT.EOL) 865 NOT EOL GO TO 800
1 214. CPH(1) = CPEF
1 215. GAMPA(1) = CPEF/(CPRF-1./MM(1))
1 216. IT = IT+1
1 217. IPI = 1
1 218. NPI = 1
1 219. CALL SAVE
1 220. EOL = .FALSE.
1 221. EPI = 1./MM(1)
1 222. GO TO 334
1 223. 907 NPI = 1
1 224. 865 WRITE(JOUT,865)
1 225. IF (ISV) CALL SAVE
1 226. 898 IT = IT+1

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• ROCK0008

• ROCK0121

ROCKET

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PAGE 5

227. IF 11.6E, M1) GO TO 999

228. 11 = 11.1

229. 11 = 11.11

230. GO TO 372

231. 999 IF 11.6E, M1) RETURN

232. GO TO 321

233. END

• POCRC179

END FILE 887 18ANK 305 011111 1382 COMMON

ENDOG, P READ

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RPEAD

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25IN,S READ,RPEAD
FTN 9P,1200:/14/81-16:34,12.1
SUBROUTINE RPEAD(FIRST)
1. LOGICAL FIRST
2.
3. C
4. C
5. C DATA ARRAYS FOR REACTANT CARDS
6. CHARACTER NAME(16)
7. DIMENSION NAME(25,6),ANUM(25,6),PECMT(25,6),MOLE(25),ENTH(25),
8. X FAZ(25),RTMP(25),FOX(25),DENS(25)
9. COMMON /CCC/GEAFH,JOUT,DEMAND
10. C
11. C COMMON /CFUEL/CF
12. C ARRAYS FOR DATA MENU'S
13. CHARACTER*4 YES,YYES,PLANK
14. DATA BLANK/' '
15. DATA YES/'YES'
16. DATA N3/B/LNB/32/
17. DATA TBLANK/' ',LAST/' ',I2ZER0/'00'
18. C
19. C CALL NEWPAG
20. C TO=M3
21. C 6 NRFAC=0
22. C
23. C FOR FIRST PASS DO NOT CHECK SAVED DATA
24. C IF(.NOT.FIRST) GO TO 10
25. WRITE (JOUT,10000)
26. FORMAT (1,1,YE TO READ IN PREVIOUS REACTANT SET')
27. READ (5,10002) YYES
28. READ (5,10002) YYES
29. IF (YES.NC.YYES) GO TO 50
30. C
31. C READ IN PRESENT CASE
32. C 10 CONTINUE
33. IF (IO.EQ.N3) PERIOD IO
34. READ (IO) NRFAC,CF
35. C
36. C IF(NRFAC.LT.1) GO TO 50
37. C DO 25 Y=1,NRFAC
38. READ (IO) (NAME(I),J),ANUM(I),J,J=1,5),PECMT(I),MOLE(I),
39. ENTH(I),NRFAC(I),ANUM(I),6),FAZ(I),RTMP(I),FOX(I),DENS(I)
40. CONTINUE
41. C
42. C DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST)
43. C 50 CONTINUE
44. C CALL NEWPAG
45. C IF (NRFAC.LT.1) GO TO 70
46. C WRITE (JOUT,10010)
47. C 10010 FORMAT (1,1,NCFH'.2N',REACTANT'.2N',DEL WT'.3N',
48. X MOLE'.2N',ENTH'.2N',FAZ'.2N',RTMP'.2N',FOX'.2N',DENS'.2N',
49. X 2X,DENSITY'.6N',40 MOLES'.8N',INT ENERGY'.18N',OXID')
50. C DO 60 I=1,NRFAC
51. C WRITE (JOUT,10020)
52. C IF (NAME(I).EQ.I2ZER0) NAME=JAST
53. C WRITE (JOUT,10020) I,NAME(I),J,ANUM(I),J,J=1,5),PECMT(I),MOLE(I),
54. X ENTH(I),FAZ(I),RTMP(I),FOX(I),DENS(I)
55. C 60 CONTINUE
56. C WRITE (JOUT,10020)

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RREAD

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56. 10020 FORMAT (1,175X,'8.8X',INDICATES ENTHALPY TO BE CALCULATED)
57. 70 CONTINUE
58. WRITE (JOUT,100001)
59. 10030 FORMAT (1, TYPE 1 TO MODIFY, 2 TO DELETE, 3 TO ADD A REACTANT)
60. X, TYPE 0 TO CONTINUE)
61. 10010
62. READ (5,*) IOPT
63. IF (IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70
64. IF (IOPT.EQ.0) GO TO 400
65. GO TO 190,90,300,1007
66. C
67. C SELECT REACTANT NUMBER
68. 90 CONTINUE
69. N=1
70. IF (NREAC.EQ.1) GO TO 95
71. N=0
72. WRITE (JOUT,100001)
73. 10040 FORMAT (1, TYPE REACTANT NUMBER)
74. READ (5,*) N
75. IF (N.LT.1 .OR. N.GT.NREAC) GO TO 90
76. 95 CONTINUE
77. IF (IOPT.EQ.2) GO TO 200
78. C
79. C SELECT MODIFICATION OPTIONS
80. 100 CONTINUE
81. CALL NEWPAG
82. NAST=1BLANK
83. IF (NAME(1:6).EQ.12ZER0) NAST=1AST
84. WRITE (JOUT,100101)
85. WRITE (JOUT,100102) N, NAME(N), ANUM(N), J=1,5), PECT(N), MOLF(N)
86. WRITE (JOUT,100103) SAZINT, DIEMINT, FOXTAL, GENSINT
87. 10022 FORMAT (1,*)
88. WRITE (JOUT,100501)
89. 10050 FORMAT (1, 1 - REACTANT FORMULA, 2 - RFL WT/MO MOLES,
90. 3 - ENTHALPY/ENERGY/CALC, 4 - PHASE (5-L-G))
91. X=5 - TEMPERATURE (K)
92. X=6 - DENSITY (G/CM3)
93. 106 CONTINUE
94. 95. ICHNG=0
95. READ (5,*) ICHNG
96. IF (ICHNG.LT.0) GO TO 50
97. IF (ICHNG.LT.1) OR (ICHNG.GT.7) GO TO 104
98. GO TO 110,120,130,140,150,160,170,1CHNG
99. 110 CONTINUE
100. WRITE (JOUT,100201)
101. 10040 FORMAT (1, TYPE CHEMICAL FORMULA FOR REACTANT,
102. 2 - FOR EXAMPLE, 'C6H6' 1. 'C6H6' 4. 'C6H6')
103. DO 112 I=1,6
104. 105. WRITE (JOUT,100201)
105. ANUM(I)=C
106. 112 CONTINUE
107. READ (5,*) (NAME(I), ANUM(I), I=1,5)
108. DO 114 I=1,5
109. 114. RECORR (NAME(I), NAME(I)) NAME(I), I
110. 116 FORMAT (A4)
111. 117. CONTINUE

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PREFAD

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113. GO TO 100
114. C
115. CONTINUE
116. WRITE (JOUT,10070)
117. IC070 FORMAT (1, TYPE, 8F1 WEIGHT/NUMBER OF MOLES*)
118. READ (5,20) DECONTIN
119. MOLEIN=1M
120. WRITE (JOUT,10072)
121. IC072 FORMAT (1, TYPE, YES IF VALUE IS MOLES*)
122. READ (5,10002) YYES
123. IF (YYES.NE.YES) GO TO 100
124. MOLEIN=1MM
125. GO TO 100
126. C
127. CONTINUE
128. WRITE (JOUT,10080)
129. IC080 FORMAT (1, TYPE, ENTHALPY/INTERNAL ENERGY*)
130. READ (5,20) ENTMIN
131. NAMEIN=1M
132. WRITE (JOUT,10082)
133. IC082 FORMAT (1, TYPE, YES IF ENTHALPY IS TO BE CALCULATED*)
134. READ (5,10002) YYES
135. IF (YYES.EC.YYES) NAMEIN=1MM
136. GO TO 100
137. C
138. CONTINUE
139. WRITE (JOUT,10090)
140. IC090 FORMAT (1, TYPE, PHASE (S-L-G), IN A1 FORMAT *)
141. READ (5,10092) PPHIN
142. GO TO 100
143. C
144. CONTINUE
145. WRITE (JOUT,10100)
146. IC100 FORMAT (1, TYPE, TEMPERATURE (K*))
147. READ (5,20) TEMPMIN
148. GO TO 100
149. C
150. CONTINUE
151. WRITE (JOUT,10110)
152. IC110 FORMAT (1, TYPE, EXHAUSTION INDEX IF (0), IN A1 FORMAT *)
153. READ (5,10092) EXHAUSTION
154. GO TO 100
155. C
156. CONTINUE
157. WRITE (JOUT,10120)
158. IC120 FORMAT (1, TYPE, DENSITY (G/CC*))
159. READ (5,20) DENSIN
160. GO TO 100
161. C
162. DELETE A REACTANT
163. CONTINUE
164. NAMEIN=1M
165. MOLEIN=1M
166. IC020 FORMAT (1, TYPE, REACTANT)
167. READ (5,20) REACT
168. NAMEIN=1M
169. MOLEIN=1M

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READ

A-94

PRE AD

87-01-09

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22A. C
229. C STORE CASE TO FILE B
230. CONTINUE
231. REMIND 10
232. IF 110.NE.NB1 GO TO 408
233. NO 406 1=1.5
234. READ 1101 ADUMMY
235. CONTINUE
236. 406
237. CONTINUE
238. WRITE 1101 NPEAC,CF
239. DO 410 1=1,NPEAC
240. WRITE 1101 (NAME(1,J),ANUM(1,J),J=1,*,PECUT(1),MOLE(1),
241. ENTH(1),NA-E(1,6),ANUM(1,6),FAZ(1),RTEMPL(1),FOR(1),DENS(1))
242. CONTINUE
243. IF 110.EQ.NB1 GO TO 420
244. WRITE 1101 ADUMMY
245. 1113D FOR 1101 TYPE YES TO EDIT COAL REACTANT DATA
246. READ 15,10002) YES
247. IF 1YES.NE.YES) GO TO 420
248. 10=N8
249. REMIND 10
250. NO 412 1=1.5
251. READ 1101 ADUMMY
252. CONTINUE
253. 412
254. 60 TO 10
255. ENDFILE 10
256. RETURN
257. 420
258. 420 ENDFILE 10
259. 402 FOR 411,112,2,11
260. 402 FOR 411,112,2,11
261. 402 FOR 411,112,2,11
262. 402 FOR 411,112,2,11
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413. 402 FOR 411,112,2,11
414. 402 FOR 411,112,2,11
415. 402 FOR 411,112,2,11
416. 402 FOR 411,112,2,11
417. 402 FOR 411
```

SAVE

DATE 051001

PAGE

1

Q IN 5 SAVE:SAVE

FTN 0912005/14/01-16:30(16.1)

1. SUBROUTINE SAVE
2. C
3. C SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES
4. C

5. COMMON /MOLCON/ INTRGHS,IT,ITZTWO,INTRMPCON,ITZERO

6. INCLUDE SPECR.LIST

7. COMMON /SPECES/ EN(150),I,ENLM(150),S(1),O(1),H(1),O(1),DELM(150),

8. SUB(150),I,USE(150),SLM(150),TEMP(50),21

9. COEF(12,7,150),R(25,150)

10. COMMON /MISC/ ENN, SUMN, IT, SN, ATOM(1,101),LLMT(25),BO(25),

11. BOPI(25,2),TM,TLOW,THID,THIGH,PP,CPSUM,OF,FORMAT,

12. MSURD,AM(2),MPP(2),RM(2),VM(2),VPLS(2),VPI(2),

13. DATA(25),AML,CPRI,NAME(25,6),ANUM(25,6),PECNT(25),

14. ENTH(25),FAZ(25),PTEMP(25),FOX(25),DEN(25),RMOP,

15. RPI(25),TLM,ORF(26),ENML,FMSAVE,ENLSAV

16. COMMON /INDX/ IDEBUS,CONVE,IP,MP,SP,ISV,MOLES,MP,NT,NPT,MLM,MS,

17. KPAT,IMAT,IOI,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLIO,

18. NFEAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE

19. COMMON /CCC/ GRAPH,JOUT,DEMAND

20. COMMON /CFUEL/CF,HMVW,WCR,PER,CCR

21. LOGICAL IONS

22. C
23. C NEXT POINT IN SCHEDULE. USE PREVIOUS COMPOSITIONS FOR THIS T
24. IF (IOT) GO TO 13
25. ENN = ENSAVE
26. ENML = ENLSAV
27. LL1 = NLM

28. DO 50 J = 1,NS

29. IF (IOT) IONS = OP,LLMT(NLM),EQ,LSAVI GO TO 15

30. IF (LLMT(NLM),EQ,IE) GO TO 13

31. IF (IUSE(IJ),NE,-10000) GO TO 15

32. IUSE(IJ) = 0

33. LL1 = NLM+1

34. GO TO 20

35. IF (ISLMIJ),NE,-5,OP,IUSE(IJ),NE,0) GO TO 15

36. LL1 = NLM-1

37. IUSE(IJ) = -10000

38. GO TO 50

39. IF (IUSE(IJ),EC,PI GO TO 20

40. EN(IJ,MPT) = SLM(IJ)

41. IF (IUSE(IJ),GT,0) IUSE(IJ) = - IUSE(IJ)

42. IF (EN(IJ,NPT)) .GT. 0.0) IUSE(IJ) = - IUSE(IJ)

43. GO TO 50

44. EN(IJ,MPT) = 0.

45. EN(IJ,NPT) = SENTJ

46. IF (EN(IJ,NPT)) .GT. 0.0) .LE. ENML GO TO 5

47. EN(IJ,MPT) = EXP(ENML(IJ))

48. SC CONTINUE

49. NLM = LL1

50. RETURN

51. C FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T

52. IOT ISV = -ISV

SAVE

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53. 10SAVE = 101
54. ENSAVE = ENM
55. ENLSAV = ENML
56. LSAVE = LLMTIM(M)
57. DO 150 J = 1,NS
58. SLN(J) = ENL(J)
59. 150 IF (I150(J) .NE. 0) SLN(J) = ENL(J,TSV)
60. C USE COMPOSITIONS FROM PREVIOUS POINT
61. 200 DO 100 J = 1,NS
62. 100 EN(J,MP1) = ENL(J,TSV)
63. RETURN
64. END

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END FTM 161 IBANK 19 DBANK 10260 COMMON

SHOG.P SEARCH

SEARCH

DATE 051401

PAGE 1

OF 14.5--SEARCH,SEARCH

FIN 01M2005/14/01-16:14122.1

SUBROUTINE SEARCH

2. C SEARCH TYPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED

3. C COMMON /MOLCON/ ENDGAS,IF,IZPRO,IMR,MTC,OF,ZERO

4. C INCLUDE SPECIES LIST

5. C COMMON /SPECIES/ EN1150,11,ENL1150,511,01,MD1150,DE1150,1

6. C SUP1150,31,USE1150,51,MD1150,TEMP150,21

7. C COEF11,7,150,1,125,150

8. C COMMON /MISC/ ENN,SUM,11,50,ATOM13,101,ALLM125,1,00125,1

9. C BOP125,21,FM125,FMID,FMIG,PP,CPSUM,OF,OPAT,

10. C HSURD,AM121,MP121,PM121,VH121,VPLS121,MP121,

11. C DATA125,1,AM1,CP1,NAME125,61,ANUM125,61,PECUT125,1

12. C ENTH125,1,FAZ125,1,RTEMP125,1,COI125,1,DEMS125,1,PMOP,

13. C RMV125,1,TLN,OFF126,1,ENML,FMSAVE,ENLSAV

14. C COMMON /INDX/ JCEBUEALCONV,1,HP,SE,1,SE,MOLES,MP,NJ,MP1,L,MS,

15. C KMAT,IMAT,101,NOF,NOH1,1,1,NEVR,IOMS,MC,J50L,JL10,

16. C MPEAC,IC,J51,VOL,SHOCH,IT,NEZ,CALCH,IOSAVE,LSAVE

17. C COMMON /CCC/ GRAPH,JOUT,DEMAND

18. C DIMENSION O(1),DATE(12,3),MT(1),OMIT(1,3,3)

19. C EQUIVALENCE (DATE,SI,TEMP,OMIT)

20. C INTEGER ENDGAS,OMIT,PMFZ,SUB

21. C LOGICAL NEWP

22. C CHANGE WHEN CHANGE SPECIES SIZE

23. C NSPPI=150

24. C NC=0

25. C IF=0

26. C SUB(1,1)=END

27. C NEWINC=0

28. C DO 3 I=1,150

29. C DO 3 J=1,L

30. C A(I,J)=0.0

31. C READ(4,51) TLOW,TPID,INTGM

32. C 5 FORMAT(13F10.3)

33. C WS=1

34. C 7 READ

35. C 1 J=1,41,PMFZ,11,12

36. C 10 FORMATT(AR,2A1,4A2,E1,01,AL,2F10.3)

37. C IF(1)SURINS,11,CO,END GO TO 171

38. C READ

39. C 20 FORMAT(15E15.4)

40. C IF(NOMIT,CO,0) GO TO 81C

41. C DO POS 1=1,MDPIT

42. C CO AOS J=1,3

43. C 800 IF (OMIT(I,J),.ST. SUBINCS:JIT GO TO 800

44. C 20 TO 7

45. C RCS CONTINUE

46. C 810 DO A20 M=1,4

47. C IF(PIPI,EC,M) SC TO 925

48. C DO 168 I=1,1

49. C 168 IF (ILLP111),FC, MT(1) GO TO 820

50. C DO A10 J=1,1

51. C

52. C

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SEARCH

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7  ST. 819 PRINT = 0
1  50. GO TO 7
1  51. P20 ALLANIS PERI
1  52. P25 JUSCINS = 0
53. IF P25.EC.GAS GO TO 170
54. MC = NC-1
55. TAPPINGC11 = 11
56. TAPPINGC21 = 12
57. IR = 11.1
58. IF IUSCINS-11.EC.O .OR. MC.EC.11 GO TO 145
59. ON 83F 1:1,1
60. P30 IF (141,MS1,MC,ALLANS-11) GO TO 145
61. IR = 11.1
62. 145 JUSCINS = -11
63. 170 MC = MS+1
64. IF INSOLE.NSP11 GO TO 7
65. WRITE (JOUT,871)
66. 871 FORMAT (//20H,50 DIMENSIONS IN /SPECIES/ FOUND TO BE TOO SMALL IN S
70. SEARCH)
71. 171 MS = MS-1
72. NEWB = .FALSE.
73. WRITE (JOUT,172)
74. 172 FORMAT (20H SPECIES BEING CONSIDERED IN THIS SYSTEM )
75. DO 176 1:1,MS1
76. N = 1.0
77. IF (INS.LY. N) N = MS
78. 176 WRITE (JOUT,176) (DATE11,JI,DATE12,JI,SUB1J,21,SUB1J,31,
79. SUB1J,41)
80. 176 FORMAT (15H,203,2X,3001)
81. WRITE (JOUT,88)
82. IF (JOUT.EC.6) PAUSE
83. CECT NEWB
84. RETURN
85. END

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END OFM 237 10AMP 230 DPAN 10255 CCMCM

406.P SMC

SHCK

DATE 051981

PAGE 2

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1 56. 18 NAMELIST=61:12EQ
57. CALL NEWPAG
58. WRITE (6,10000)
59. 10000 FORMAT (A, TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST*)
60. READ (5,10002) YES
61. 10002 FORMAT (A9)
62. IF (YES.EQ.YYES) WRITE (6,SHKINP)
63. WRITE (6,10010)
64. 10010 FORMAT (A, ENTER NAMELIST SHKINP INPUT *)
65. READ (5,SHKINP)
66. WRITE (6,SHKINP)
67. SEQL = INCDEQ
68. IF (T(1) .LE. 0.0) T(1) = PTEMP(1)
69. DO 20 J = 1,13
70. IF (MACH(1)) .LE. 0.0 .AND. U(1)) .LE. 0.0) GO TO 21
71. 20 NSK = 1
72. 21 10F = 10F+1
73. 22 = ORF(10F)
74. CALL NEWOF
75. INCDEQ = SEQL
76. 17 PP = P(1)
77. IT = T(1)
78. IF (INCDEQ) GO TO 19
79. C FROZEN
80. DO 11B I = 1,13
81. DLV(P(1)) = 1.0
82. 11B DLVPT(1) = -1.0
83. 19 DO 15 NPT = 1,24
84. TTT(NPT) = T(NPT)
85. IF (NPT.EQ.1) GO TO 14
86. IF (TTP(NPT)) .LE. 0.0) PTP(NPT) = PTP(NPT)-17
87. IF (TTT(NPT)) .LE. 0.0) TTT(NPT) = TTT(NPT)-1)
88. SSUM(NPT) = SSUM(NPT)-1)
89. HSUM(NPT) = HSUM(NPT)-1)
90. IF (TTT(NPT).EQ.17.AND.PTP(NPT).EQ.17) GO TO 15
91. 14 PP = PTP(NPT)
92. 15 PP = PTP(NPT)
93. CALL MCALC
94. HSUM(NPT) = "SUBC
95. IF (CPRI.GT. 0.0) GAMMA1 = CPRI/(CPRI - 1.0/AM1)
96. IF (GAMMA1.GT. 0.0) GO TO 38
97. WRITE(JOUT,16)
98. IF (FORMAT 17720,MISSING GAMMA1 OR CP VALUE IN SHCK)
99. RETURN
100. 38 A1 = SQRT(PP*GAMMA1*TT/A01)
101. IF (U(NPT) .LE. 0.0) U(NPT) = A1*MACH(NPT)
102. IF (MACH(NPT)) .LE. 0.0) MACH(NPT) = U(NPT)/A1
103. M(NPT) = AM1
104. CPRINT = CPRI
105. 39 GAMMA(NPT) = GAMMA1
106. ECL = .FALSE.
107. C OUTPUT--1ST CONDITION
108. WRITE(JOUT,861)
109. 861 FORMAT(1H,13X,CONTRIBUT SHCK HAVE PARAMETERS ASSUMING
110. IF (.NOT. INCDEQ) GO TO 44
111. WRITE(JOUT,862)
112.

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SMCM

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113.      B62 FORMAT (1H,51X,23H'EQUILIBRIUM COMPOSITION '//)
114.      GO TO 45
115.      WRITE (JOUT,P63)
116.      B63 FORMAT (1H,52X,18H'FROZEN COMPOSITION '//)
117.      AS CALL OUT1
118.      WRITE (JOUT,P64)
119.      B64 FORMAT (1H,51X,23H'INITIAL GAS (1) ')
120.      FM(3) = F13
121.      FM(4) = FOUR
122.      WRITE (JOUT,FMT) FM,F6,(MACH(I),J=1,NPT)
123.      FM(4) = TWO
124.      WRITE (JOUT,FMT) FM,FUEL,(U(I),J=1,NPT)
125.      CALL OUT2
126.      C      BEGIN CALCULATIONS FOR 2ND CONDITION
127.      IF (INCODE) FOL = .TRUE.
128.      NPT = 1
129.      B7 GAMMA1 = GAMMA(INPT)
130.      P1 = PM(INPT)
131.      P1 = PPP(INPT)
132.      Y1 = Y1(INPT)
133.      MS = MSUM(INPT)
134.      P21 = 12.0*(GAMMA1*MACH1(INPT)**2-GAMMA1*1.1)/(GAMMA1*1.1)
135.      T21 = P21*12.0/(MACH1(INPT)**2-GAMMA1*1.1)/(GAMMA1*1.1)
136.      IF (11+T21-G1*2000.0-AND. EQL) T21 = .7*T21 + 600.0/T1
137.      MU12RT = AM1*U(INPT)**2/(RBR*11)
138.      P21L = ALOG(P21)
139.      T21L = ALOG(T21)
140.      P21 = 10**P21L
141.      T21 = 10**T21L
142.      P = P21*P1
143.      I = (.NOT. EQL) GO TO 40
144.      CALL EQLERR
145.      GO TO 50
146.      C FROZEN
147.      40 T1N = PLOG (T1)
148.      CALL MCALC
149.      MSUM(INPT) = MSURD
150.      CPR(INPT) = CPRI
151.      SD RM012 = M1*12/(MM(INPT)+P21)
152.      GG = RM012*MU12RT
153.      G11,112 = GG*DLVPT(INPT)-P21
154.      G11,212 = GG*DLVPT(INPT)
155.      G11,312 = 21-1.1*MU12RT*(RM012-1.1)
156.      GG = (U1(INPT)+G12)*2/RPR
157.      G12,112 = GG*DLVPT(INPT)+11*(OLVTP(INPT)-1.1)/(MM(INPT)
158.      G12,212 = GG*DLVPT(INPT)-11*(CPR(INPT)
159.      G12,312 = MSUM(INPT) - MS - U1(INPT)**2*1.0 - RM012**2/(12.0*PBR)
160.      X131 = G11,112*G12,21-G11,21*G12,112
161.      X132 = (G11,312*G12,21-G12,312*G11,21)/(X131)
162.      X121 = (G11,112*G12,31-G12,112*G11,31)/(X131)
163.      AX = X111
164.      AXH = X121
165.      IF (AX,LT,C.) AX = -AX
166.      IF (AXH,LT,C.) AXH = -AXH
167.      IF (AXH*612AY) AY = AXH
168.      IF (AY,LT,.00025) GO TO 150
169.      AY = AY/4000452

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1 170. 14 APR 68 12:00 00 00 05
1 171. 111 = 111/87
1 172. 112 = 112/87
1 173. 75 121 = 121/87
1 174. 121 = 121/87
1 175. 121 = 121/87
1 176. 121 = 121/87
1 177. 121 = 121/87
1 178. 125 125 = 125/87
1 179. 125 125 = 125/87
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1 224. 125 125 = 125/87
1 225. 125 125 = 125/87
1 226. 125 125 = 125/87

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SMCA

DATE 051001

PAGE 5

1 227. 999 RICHPIA1 = 1111

228. RETURN

229. END

END FTM 715 IRANK 568 DRANK 11567 COMMON

2NDG,P TAPESAVE

2PRT,S TAPESAVE

FURPUR 28RIW1 E1A 570111 05/19/01 16134117

SHCM

1 227. 999 PTEMPIK) = T11)
 228. RETURN
 229. END

END FTA 715 IBANK 568 DRANK 11567 COMMON

ANDG,P TAPESAVE

SPRT,S TAPESAVE
 FURPUR 2881H1 E36 S74T11 05/14/81 16134117

TAFESAVE

5FV1ENB1N2DB,IFF&10,IAFESAVE

- 1 @ASG,TF LEWISTAPE,UQS,SAVEON . LEWIS CHEM EQUIL
- 2 @COPY,GM LEWIS,,LEWISTAPE.
- 3 @COPY,GM 4,,LEWISTAPE.
- 4 @COPY,GM 8,,LEWISTAPE.
- 5 @COPY,GM 10,,LEWISTAPE.
- 6 @COPY,GM 12,,LEWISTAPE.
- 7 @XCT MIRADS,TPNO
- 8 LEWISTAPE
- 9 @FREE LEWISTAPE.

SHDG,F THERMP

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GETIN,S THERMP,THERMP

FIN 9R1H2R05/14/81-16:34129,I

1. SUBROUTINE THERMP

2. C

3. COMMON /CONST/ ATNQ,CHTT,PATM,RRAP,RRP,RVR

4. COMMON /POINTS /MSUM(13),SSUM(13),CPR(13),OLVPT(13)

5. 1,GAMMA(13),T(26),T(26),V(13),PP(13),VM(13),SONVEL(13),TTT(13)

6. 2,VLM(13),TOTK(13)

7. COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(25),

8. BOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EORAT,

9. MSURD,AM(2),HPP(2),VMIN(2),VPL(2),WPI(2),

10. DATA(25),AMI,CP(1),NAME(25,6),ANUM(25,6),PECW(25),

11. ENTH(25),FAZ(25),PTEMP(25),FOX(25),DENS(25),PHOP,

12. RM(25),TLN,OXF(26),ENN,FSN,SAVE,ENLSAV

13. COMMON /INDX/ IDERUG,CONVG,TP,HP,SP,ISV,MOLCS,NP,NT,NPT,NLM,NS,

14. MMAT,IMAT,IQ1,NOF,NOMIT,IF,NEW,IONS,INC,JSOL,JL1Q,

15. NFEAC,IC,JSI,VOL,SMOCH,IT,NF2,CALCH,IOSAVE,LSAVE

16. COMMON /OUP1/ FOX,F13,FA,FAP(2),FB,FC,F(3),FCST(2),ELV,EG(2),

17. FGE,FGV,FM(2),FT(2),FV(2),FM(2),FMT(15),FN(2),FOUR,

18. FP,FS(2),FSV,FT(2),FTN(2),FV(2),FVEL(2),ONE,THREE,

19. TWO,ZERO

20. C

21. COMMON /CCC/ GRAPH,JOUT,DEMAND

22. C

23. LOGICAL QT

24. COMMON /QUENCH/QT,IQ1,TPF,IQT,TA

25. COMMON /VEL/VEL,PHV

26. COMMON /PLT/PLT,AS,13,IPLT,IPLOT,NS,PLT

27. CHARACTER*6 FUA,FUB

28. LOGICAL HP,SP,TP,VOL

29. DATA FUA/6HU CAL//,FUB/6HGRAM /

30. C

31. IF (IT1) .LE. 0.0) Y(1) = 3800.0

32. ICF = 0

33. 95 ICF = ICF+1

34. CF = OXF(10F)

35. CALL MEMOF

36. SET ASSIGNED F OR VOLUME

37. DO 871 IP = 1,NP

38. PP = P(1P)

39. VLM(NPT) = P(1P)

40. SET ASSIGNED T

41. DO 871 IT = 1,NT

42. TT = T(IT)

43. CALL EQLBEM

44. IF (IT) .GT. 0.0) GO TO 800

45. IF (NPT .EQ. 0) RETURN

46. ISV = 0

47. IF (IP .EQ. NP .AND. IT .EQ. NT .OR. IT .LE. 0.0) GO TO 860

48. ISV = NPT

49. IF (NPT .NE. 13) GO TO 870

50. RED CONTINUE

51. IF (JOUT .EQ. 6) PAUSE

52. CALL NEWFAG

53. WRITE (JOUT,5)

54. 5 FORMAT(1H141),LENTHERMP,DYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED . MOL10072

55. 1)

THERMP

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56. IF (.NOT. VOL1) GO TO 861
57. IF (MP) WRITE(JOUT,10)
58. 10 FORMAT(1H0,62X,7H VOLUME /)
59. IF (TP) WRITE(JOUT,11)
60. 11 FORMAT(1H0,54X,22H TEMPERATURE AND VOLUME /)
61. IF (SP) WRITE(JOUT,12)
62. 12 FORMAT(1H0,54X,18H ENTROPY AND VOLUME /)
63. GO TO 862
64. 861 IF (.NOT. QTYPE.EQ.1) GO TO 18
65. IF (MP.AND. QTYPE.EQ.1) WRITE (JOUT,880)
66. 880 FORMAT (10',57X,'QUENCH ENTHALPY')
67. IF (TP.AND. QTYPE.EQ.2) WRITE (JOUT,882)
68. 882 FORMAT (10',55X,'QUENCH TEMPERATURE')
69. GO TO 862
70. 18 IF (MP) WRITE (JOUT,20)
71. 20 FORMAT(1H0,62X,10H PRESSURES /)
72. IF (TP) WRITE (JOUT,21)
73. 21 FORMAT(1H0,53X,24H TEMPERATURE AND PRESSURE /)
74. IF (SP) WRITE (JOUT,22)
75. 22 FORMAT(1H0,55X,20H ENTROPY AND PRESSURE /)
76. 862 CALL OUT1
77. WRITE(JOUT,863)
78. 863 FORMAT (25H THERMODYNAMIC PROPERTIES /)
79. IF (.NOT. VOL1) GO TO 864
80. FMT(3) = ONE
81. IF (.NOT. MP) GO TO 864
82. DO 83 I=1,NPT
83. FMT(I,2) = TWO
84. IF (I.EQ.13) FMT(15) = 5H P,2)
85. 63 VII = 58.13
86. 864 CALL OUT2
87. WRITE(JOUT,EMT) FUA,FUB,FB,(VII), I = 1,NPT)
88. CALL OUT3
89. IF (CF.EQ.1.0) ,902.
90. 900 CALL OUT4
91. 902 CONTINUE
92. IF (IPLOT.EQ.0) GO TO 910
93. DO 906 I=1,NPT
94. IJ=IPLT+1
95. WRITE (11,IJ) (PLMT(J,1),J=1,45)
96. CONTINUE
97. IPLT=IPLT+NPT
98. 910 CONTINUE
99. IF (JOUT.EQ.6) PRUSE
100. CALL NEWPAG
101. IF (ISV.EQ.0.AND.10F.EQ.NOF) RETURN
102. IF (IDEBUG.GT.13) IDEBUG=IDEBUG+13
103. WRITE(JOUT,866)
104. 866 FORMAT(1H1)
105. IF (INT.EQ.1.AND.NP.EQ.1) GO TO 95
106. NPT = 0
107. 870 NPT = NPT + 1
108. IF (.NOT. TP) TIII=TI
109. IF (TP.EQ.1.AND.T7.EQ.1) TSV=TSV
110. IF (INT.EQ.1) GO TO 871
111. IF (IT.EQ.1) ISV=0
112. 871 CALL SAVE

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* VOLIND37
 * 12-22
 * 12-22

THEMP

113.

GO TO 95

114.

END

END FIN 293 IBANK 213 DRANK 1877 COMMON

SHUG.P VERPMT

DATE 051481

PAGE

3

• MOLIND45

06TH05--VARFMT+VARFMT
RTN 98142005/14/81-16:34(10,1)

SUBROUTINE VAEFMT(V,NPT)

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2. CHARACTER*6 F9X,F13,FA,FB,FC,FCV,FMT,FOUR,FP,
3. X ONE,THREE,TWO,ZERO,F,FSV,FGE,FVG
4. CHARACTER*6 FG,F1,FIV,FI,FI1,FAP,FCP,FCST,FH,FS,FTW,FN,FVEL
5. DIMENSION FG(2),FI(2),FI1(2),FM(2),FI12(1),FI(2),FAP(2),FCPI(2),
6. X FCST(2),FHI(2),FSI(2),FTW(2),FM(2),FVEL(2)
7. COMMON /OUP1/F9X,F13,FA,FAP,FB,FC,FCP,FCST,FCV,FG,
8. X FGE,FGV,FH,FI,FI1,FM,FMT,FS,FN,FOUR,
9. X FP,FS,FSV,FI,FTW,FV,FVEL,ONE,THREE,TWO,ZERO
10.
11. DIMENSION V(13)
12. CHARACTER*6 FFOUR,FONE,FTHREE,FTWO,FZERO
13. DATA FFOUR/SHF9.4//,FONE/SHF9.3//,FTHREE/SHF9.3//,FTWO/SHF9.2//,
14. FZERO/SHF9.0//

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7. 00 45 I = 1, MPT
15 17 00 18 00 TO 40

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1. IF (I10.E2.13) GO TO 4
2. FMT(I+2) = FOUR
3. IF (VII) .GE. 10.0) FMT(I+2) = THREE
4. IF (VII) .GE. 100.0) FMT(I+2) = TWO
5. IF (VII) .GE. 1.0E4) FMT(I+2) = ONE
6. IF (VII) .GE. 1.0E6) FMT(I+2) = ZERO
7. GO TO 45
8. FMT(I5) = FFOUR
9. IF (VII) .GE. 10.0) FMT(I5) = THREE
10. IF (VII) .GE. 100.0) FMT(I5) = TWO
11. IF (VII) .GE. 1.0E4) FMT(I5) = ONE
12. IF (VII) .GE. 1.0E6) FMT(I5) = ZERO
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1. RETURN
2. END

END FIS 144 IBANK 69 DRANK 87 COMMON

613

ORIGINAL PAGE IS
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REUNION DE LEVISEY ACCY IMPROBES007I 120058104MI ISSR ASINJ7 IOIMNO
BOZMIGIAVES I A3JCPO4 PROCTY SEVIGNBIMZOR

LO#D 13252 TR3 PUP -1 LEWIST

LEWIS RIN

Time: TOTAL: 00:02:45.746 CB5155: 033039822

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CPU: 00:00:14.784  I/O: 00:01:35.287
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CC/EB: 00:00:50.674
WAIT: 00:00:07.924

IMAGES READ: 07 PAGES: 111

DATE 051481

VACANT

START: 16:28:11 MAY 14, 1981 FIN: 16:24:22 MAY 14, 1981

.....
 INITIAL USE OF LABELED FRBC TAPES HAS IDENTIFIED A PROBLEM
 PLEASE DISCONTINUE USE OF LABELED FRBC TAPES UNTIL FURTHER NOTICE

$123456789 \sim 123456789^{(1)} 123456789^{(2)} 123456789^{(3)} 123456789^{(4)} 123456789^{(5)} 123456789^{(6)} 123456789^{(7)} 123456789^{(8)} 123456789^{(9)}$

A-112

APPENDIX B

SOURCE LISTING OF PROGRAM ELEMENTS WITHOUT MODIFICATION

This is a printout of the Lewis Chemical Equilibrium Program without the modification required for multiple runs. Note that this material is identical to the after modification listing (Appendix B) of "Addition to the Lewis Chemical Equilibrium Program to Allow Computation from Coal Composition Data."

[illegible]

BARUN L. WIST, 14 PA 01950021, SEVIGNBIN209, 30,200

MSG,N REMOVE AT CARD READER 10-15-80 CLOCK NO 2,09

BASE, 1 PUR, UOS, 1575, 9

3 COPY, 6 PUR., 1 P. 5.
FURUR 28RMI 33 57011 10/15/80 13:09:46
SEVENHIN20-LEWIS11 COPIED ON 09/18/80 13:23:53
105 BLOCKS COPIED.
FOR ENCOUNTERED ON INPUT TAPE

3XQT, A SVS80MSFC9.LISYIT

AND, P. A.

APR 15 1962 10:05:53

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SEVIGNBIN208+TPFS(0).A
1 LIB LEWIS. MI. ILIB. SYS. MSF.
2 SEG DRIVER,
3 IN LEWIS. BLOCK1
4 IN LEWIS. MAIN
5 SEG 00*(DRIVER)
6 IN LEWIS. COALCV
7 SEG 1*(DRIVER)
8 IN LEWIS. SEARCH
9 SEG 2*(DRIVER)
10 IN LEWIS. REACT
11 SEG 3*(DRIVER)
12 IN LEWIS. THERMP
13 SEG 4*(DRIVER)
14 IN LEWIS. DETON
15 SEG 5*(DRIVER)
16 IN LEWIS. SHCK
17 SEG 6*(DRIVER)
18 IN LEWIS. ROCKET
    
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3HDS.P BLOCK1

ORIGINAL PAGE IS
OF POOR QUALITY

8FOP+S BLOCK1,BLOCK1
HSA E3 -10/15/80-13:05:54 (11.)

BLOCK DATA

STORAGE USED: CODE(1) 000000; DATA(0) 000000; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCON 000010
0005 MISC 001701
0006 OUP 000073

STOP ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

BLOCK	TYPE	RELATIVE LOCATION	NAME
0005	000680 AM	000705 AM1	0005 001135 ANUM
0003	000000 ATMN	0005 000514 BO	0005 000235 ATEM
0005	000634 CP SUM	0005 001560 DENS	0005 000706 CPRI
0005	000000 ENN	0005 001677 ENSAVE	0005 001700 ENLSAV
0006	000002 FA	0005 001845 FAZ	0005 000636 EORAT
0006	000007 FCP	0006 000014 FCV	0005 000006 FC
0006	000020 FGV	0006 000023 FI	0006 000017 FGE
0006	000031 FMT	0006 000032 FOUT	0006 000027 FM
0006	000054 FS	0006 000037 FT	0006 000053 FP
0006	000065 FVEL	0006 000000 F9X	0006 000063 FV
0005	000642 HPP	0004 000001 F13	0003 000001 GMET
0005	000463 LLMT	0005 000637 HSUBO	0004 000003 IZER0
0005	000006 OX	0004 000005 MOL	0005 000635 OF
0003	000003 RBAP	0005 001644 OXF	0005 001363 PECVI
0005	001476 RTEMP	0003 000004 RBR	0005 001611 PHOP
0006	000070 THREE	0003 000005 RVR	0005 000632 THIGH
0005	000002 TT	0005 001843 TLM	0005 000631 TMID
0004	000007 ZERO	0006 000071 TWO	0005 000652 WP
		0006 000012 ZERO	

BLOCK	DATA	ATM000001
00101	1*	000000
00101	2*	000000
00102	3*	000000
00103	4*	000000
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00104	9*	000000
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00105	15*	000000
00106	16*	000000
00107	17*	000000

COMMON /CONSTS/ ATMN,GMET,PAIM,CBAR,RBR,PVR
COMMON /HOLCON/ END,GAS,IE,IZER0,LANK,MOL,OX,ZERO
COMMON /MISC/ ENN,SUM,TT,50,ATOM13,101,LLMT(25),BO(25),
BO(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EORAT,
HUBO,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),
DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECVI(25),
ENTHI(25),FAZ(25),PTEMP(25),FOX(25),DENS(25),PHOP,
PM(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV
COMMON /OUP/ F9X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FG(2),
FGE,FGV,PH(2),FI(2),FIV(2),FHI(2),FMT(15),FN(2),FOUR,
FV,FS(2),FVS,FT(2),FTK(2),FV(2),FVEL(2),FONE,THREE,
TWO,ZERO

DIMENSION ATAM(3,51),ATEM(3,50)
EQUIVALENCE (ATOM1,1,ATAM), (ATOM1,52), (ATEM)

BLOCK1

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00107 18* C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES 000000
00107 19* DATA ATOM/2HM, 1.0071, 1.0, 2HME, 4.0026, 0.0, 2HLI, 6.939, 1.0, 2HRE, 000000
00110 20* 1 9.0122, 2.0, 2HB, 10.811, 3.0, 2HC, 12.0115, 4.0, 2HM, 14.0067, 0.0, 000000
00110 21* 2 2HO, 15.0994, 2.0, 2HF, 18.9984, -1.0, 2HNE, 20.183, 0.0, 2HNA, 22.9898, 000000
00110 22* 3 1.0, 2HMG, 24.312, 2.0, 2HAL, 26.9815, 3.0, 2HJ, 28.086, 4.0, 2HP, 30.9738, 000000
00110 23* 4 5.0, 2HS, 32.064, 4.0, 2HCL, 35.453, -1.0, 2HAP, 39.948, 0.0, 2HK, 39.102, 000000
00110 24* 5 1.0, 2HCA, 40.080, 2.0, 2HSC, 44.956, 3.0, 2HTI, 47.90, 4.0, 2HV, 50.942, 000000
00110 25* 6 5.0, 2HCR, 51.996, 3.0, 2HMN, 54.9380, 2.0, 2HFE, 55.847, 3.0, 2HCO, 58.9332, 000000
00110 26* 7 2.0, 2HMI, 58.710, 2.0, 2HCU, 63.540, 2.0, 2HZN, 65.370, 2.0, 2HGA, 69.720, 000000
00110 27* 8 3.0, 2HCE, 72.590, 4.0, 2HAS, 74.9216, 3.0, 2HSE, 78.960, 4.0, 2HBR, 79.909, 000000
00110 28* 9 -1.0, 2HMR, 83.80, 0.0, 2HBR, 85.47, 1.0, 2HSP, 87.620, 2.0, 2HY, 88.905, 000000
00110 29* 3 0.0, 2H2R, 91.220, 4.0, 2HNB, 92.906, 5.0, 2HMO, 95.94, 6.0, 2HIC, 99.0, 7.0, 000000
00110 30* 8 2HRU, 101.070, 3.0, 2HRH, 102.905, 3.0, 2HPD, 106.40, 2.0, 2HAG, 107.840, 000000
00110 31* C 1.0, 2HCO, 112.40, 2.0, 2HTN, 114.820, 3.0, 2HSN, 118.690, 4.0, 2HSR, 000000
00110 32* D 121.750, 3.0, 000000
00110 33* DATA ATOM/2HTE, 127.60, 4.0, 2HI, 126.9044, -1.0, 2HKE, 131.30, 0.0, 2HCS, 000000
00112 34* 1 132.905, 1.0, 2HBA, 137.340, 2.0, 2HLA, 138.910, 3.0, 2MCE, 140.120, 3.0, 000000
00112 35* 2 2HPR, 140.907, 3.0, 2HND, 144.240, 3.0, 2HPM, 145.0, 3.0, 2HSM, 150.350, 3.0, 000000
00112 36* 3 2HEU, 151.960, 3.0, 2HGD, 157.250, 3.0, 2HTB, 158.924, 3.0, 2HJ, 162.50, 000000
00112 37* 4 3.0, 2HHD, 164.930, 3.0, 2HEP, 167.260, 3.0, 2HTM, 168.934, 3.0, 2HYB, 000000
00112 38* 5 173.040, 3.0, 2HLU, 174.997, 3.0, 2HMF, 178.490, 4.0, 2HTA, 180.948, 5.0, 000000
00112 39* 6 2HW, 183.850, 6.0, 2HRE, 186.20, 7.0, 2HOS, 190.20, 4.0, 2HIR, 192.20, 4.0, 000000
00112 40* 7 2HPT, 195.090, 4.0, 2HAU, 196.97, 3.0, 2HHG, 200.590, 2.0, 2HIL, 204.370, 000000
00112 41* 8 1.0, 2HPB, 207.190, 2.0, 2HBI, 208.980, 3.0, 2HFO, 210.0, 2.0, 2HAT, 210.0, 000000
00112 42* 9 0.0, 2HGN, 222.0, 0.0, 2HFR, 223.0, 1.0, 2HRA, 226.0, 2.0, 2HAC, 227.0, 3.0, 000000
00112 43* A 2HTM, 232.038, 4.0, 2HFA, 231.0, 5.0, 2HU, 238.030, 6.0, 2HNP, 237.0, 5.0, 000000
00112 44* B 2HPU, 242.0, 4.0, 2HAM, 243.0, 3.0, 2HCM, 247.0, 3.0, 2HBK, 249.0, 3.0, 2HCF, 000000
00112 45* C 251.0, 3.0, 2HES, 254.0, 0.0, 2HFM, 253.0, 0.0, 2HIC, 12.0115, 4.0, 000000
00112 46* INFORMATION USED IN VARIABLE OUTPUT FORMAT 000000
00114 47* DATA F9X/TH9X, F13/2HJ3, FA/6HAE/AT, FB/6H, /FC/6HCF, /, /OUP/ 000000
00114 48* 1 FCV/6HCF VAC, FG/12HGGAMMA (S), /FI/12HISP SECONDS, /, /OUP/ 000000
00114 49* 2 FIV/12HIVAC SECONDS, /FM/12HM MOL WEIGHT, /FMT/6H11H, 2, /OUP/ 000000
00114 50* 3 6HA6, A2, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 000000
00114 51* 4 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 5HF9.1, 000000
00114 52* 5 FN/12HMACH NUMBER, /FOUR/5HF9.1, /FP/6HPCP, /, /OUP/ 000000
00114 53* 6 FT/12HIDLV/DLP, Y, /FV/12HIDLV/DLP, P, /ONE/5HF9.1, /, /OUP/ 000000
00114 54* 7 THREE/5HF9.3, /, TWO/5HF9.2, /, ZERO/5HF9.0, /, FAP/12HMPRESS, N/M, 000000
00114 55* 82, FCP/12HCP CAL/IG/1K, 2H, /, FCST/12HCSTAR M/SEC, /, FGE/6HIEFF, /, 000000
00114 56* 9 FGV/6HGAS VE, /FM/12HMENTH CAL/G, /FS/12HS CAL/IG/1K, /, FSV/6HSON V 000000
00114 57* AE, FTW/12HTEMP DEG. K, /FVEL/6HL M/SEC, 2HC, / 000000
00114 58* DATA END/3HEND, 6AS/1HG, /IE/1HE, /I2ERO/2HOO, /LANK/2H, /, MOL/1HM, 000000
00153 59* 1 0X/1HO, /, ZERO/1HO, /, ATNM/101325.0, /, RVP/82.0554497, 000000
00153 60* 3 6ME/19.806650, /, PATM/14.6960060, /, RBAR/1.9871650, /, RBR/8314.29360, 000000
00153 61* END ATMD00060 000000
00172 62*

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END OF COMPILATION: NO. DIAGNOSTICS.

ENDG,P ROOT

SPRT,S ROOT

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ROOT

DATE 101580

PAGE

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2	BCAT,P	N,F/64/IRK/128	
3	BCAT,P	8,F/10/IRK/32	
4	BCAT,P	10,F/10/IRK/32	
5	BCAT,P	12,F/10/IRK/64	
6	ASG,A	LEWIS	
7	ASG,A	4	
8	ASG,A	8	
9	ASG,A	10	
10	ASG,A	12	
11	BCPY	TPFS	LEWIS
12	BCPY,G	PUR	4
13	BCPY,G	PUR	8
14	BCPY,G	PUR	10
15	BCPY,G	PUR	12
16	FREE	PUR	

CHECK

ADG,P

CHECK

FOR,S CHECK,CHECK
HSA E3 -10,15/0-13:05:57 (2,)

SUBROUTINE CHECK ENTRY POINT 000036

STORAGE USED: CODE(1) 000065; DATA(0) 000013; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 NERR3

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000 I 000000 IBLNK2 0000 I 000005 ICHAR1 0000 I 000006 ICHAR2 0000 I 000001 IHIGH 0000 I 000002 ILOW
0000 000007 INJPS 0000 I 000003 JHIGH 0000 I 000004 JLOW

00101	1*		SUBROUTINE CHECK(NAME)	000000
00101	2*	C		000000
00101	3*	C	BLANK FILL SPECIES SYMBOLS	000000
00103	4*		DATA IBLNK2/2H /,THIGH/1HZ/,ILOW/1HA/	000000
00107	5*		DATA JHIGH/O/,JLOW/O/,ICAR1/O/,ICAR2/O/	000000
00114	6*		FLD(30,6,ICAR1)=FLD(0,6,NAME)	000000
00115	7*		FLD(30,6,ICAR2)=FLD(6,6,NAME)	000001
00116	8*		FLD(30,6,JHIGH)=FLD(0,6,IHIGH)	000003
00117	9*		FLD(30,6,JLOW)=FLD(0,6,ILOW)	000005
00120	10*		IF (ICAR1.LT.JLOW .OR. ICAR1.GT.JHIGH) NAME=IBLNK2	000007
00122	11*		IF (ICAR2.LT.JLOW .OR. ICAR2.GT.JHIGH) FLD(6,6,NAME)=	000027
00122	12*	*	FLD(6,6,IBLNK2)	000027
00124	13*		RETURN	000047
00125	14*		END	000064

END OF COMPILATION: NO DIAGNOSTICS.

HDG,P COMCV

COALCV

FOR S COALCV, COALCV
HSA E3 -10,15,8-13:05:50 (24,1)

5 SUBROUTINE COALCV ENTRY POINT 003674

STORE USED: CODE(1) 003713; DATA(1) 003744; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CFUEL 000004
0004 SPECES 017106
0005 INOX 000021
0006 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0007 ROYES
0010 PAGIT
0011 CHRST2
0012 GOUT
0013 INCODES
0014 ROATAI
0015 ROATAF
0016 NREWS
0017 NREWS
0020 NI024
0021 NI034
0022 NI014
0023 NERR24
0024 NWRUS
0025 NWEFS
0026 NERR34

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000030	10L	0000	002175	100F	0001	001444	10116	0001	001477	10256	0001	000460	1041
0001	001535	1040G	0000	002205	106F	0001	001743	10736	0000	002233	108F	0001	001764	11076
0001	000537	112L	0001	002063	11376	0001	000554	114L	0001	002075	11476	0001	000607	1201
0001	002213	1204G	0001	002213	12076	0001	002246	12256	0001	002316	12456	0001	000617	1261
0001	002360	1270G	0001	002370	12736	0001	000635	130L	0001	002454	13226	0001	002531	13476
0001	002541	1354G	0001	002553	13626	0001	002565	1370G	0001	002576	13756	0001	002607	14056
0001	002653	1426G	0001	002733	14526	0001	002734	14556	0001	003021	1504G	0001	003034	15116
0001	003035	1514G	0001	003213	1550G	0001	003214	15516	0001	003283	1574G	0001	003263	15776
0001	003322	1615G	0001	003407	16426	0001	003422	16476	0001	003423	16526	0001	003564	17276
0001	003564	1731G	0001	003571	1736G	0001	003571	1740G	0001	003576	17456	0001	003576	17476
0001	003603	1754G	0001	003603	1756G	0001	003620	1770G	0001	003624	1774G	0001	000011	2056
0001	000016	2126	0000	002404	2350F	0001	001102	2352L	0000	002410	2354F	0001	001137	2357L
0001	001143	2358L	0001	001177	2360L	0001	001250	2364L	0001	001254	2366L	0001	001257	2370L
0001	001263	2372L	0001	001315	2380L	0001	001352	2384L	0001	002053	2420L	0001	002116	2422L
0000	002547	2424F	0001	002112	2427L	0001	002152	2428L	0001	002216	2431L	0001	002222	2432L
0001	002225	2434L	0001	002231	2436L	0001	000126	2566	0001	000126	2606	0001	000133	2656
0001	000133	2676	0001	000140	2746	0001	000140	2766	0001	000637	300L	0001	000145	3036

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0001 000145 305G 0001 000513 310L 0001 000660 312L 0001 000675 314L 0001 000677 316L
0001 000710 320L 0001 000716 322L 0001 000727 324L 0001 000740 326L 0001 000751 328L
0001 000762 330L 0001 000773 330L 0001 001013 342L 0001 000240 343G 0001 001017 343L
0001 001060 348L 0001 001063 350L 0001 001386 351L 0001 001366 352L 0001 001377 354L
0001 001410 356L 0001 001421 358L 0001 000273 362G 0001 001502 364L 0001 001520 366L
0001 001524 367L 0001 000302 370G 0001 001562 372L 0001 001565 380L 0001 001567 382L
0001 001600 390L 0001 002533 394F 0001 001773 400L 0001 002020 402L 0001 000335 406G
0001 000343 413G 0001 002031 420L 0001 002267 421L 0001 002301 422L 0001 002305 423L
0001 002347 428L 0001 002352 430L 0001 002405 434L 0001 002410 440L 0001 002412 442L
0001 000434 445G 0001 002423 450L 0001 002443 453L 0001 002448 454G 0001 002449 454G
0001 002501 460L 0001 002504 470L 0001 002437 452L 0001 002706 504L 0001 002706 504L
0001 000523 505G 0001 002767 520L 0001 000611 533G 0001 003070 540L 0001 000626 543G
0001 003276 552L 0001 003301 554L 0001 002020 56F 0001 003361 560L 0001 002024 58F
0001 003455 590L 0001 002032 60F 0001 002055 62F 0001 001030 620G 0001 001112 654G
0001 001122 662G 0001 003652 680L 0001 002100 70F 0001 001245 717G 0001 001245 722G
0001 001300 740G 0001 001323 751G 0001 001334 754G 0001 000316 80L 0001 002122 84F
0001 000357 90L 0001 002131 92F 0001 002193 94F 0001 011052 A 0001 002122 84F
0001 000576 94UM 0001 003461 94H 0001 001777 HHV 0001 003331 ACOMP 0001 002744 CCOMP
0001 000000 CF 0001 002732 COAL 0001 000000 COEF 0001 001640 CC 0001 002744 CCOMP
0001 001780 CTEMP 0001 010424 DELM 0001 000002 DEMAND 0001 000001 CONV6 0001 001774 CSUM
0001 010150 ENLN 0001 001447 ENTH 0001 002676 FAZ 0001 000001 DEMS 0001 004312 EN
0001 001531 FOX 0001 000000 GRAPH 0001 002001 HF1 0001 002003 HF2 0001 002000 FES2C
0001 001664 HHT 0001 000000 HHT 0001 001777 HHV 0001 000001 HHV 0001 001734 HH 0001 001734 HH
0001 001657 H2O 0001 001637 I 0001 003331 ICOMP 0001 000003 MP 0001 001734 HH
0001 001645 ICC 0001 002744 ICOMP 0001 002732 ICAL 0001 001625 ID 0001 001744 IC 0001 001744 IC
0001 001752 IE 0001 002676 IF4Z 0001 0001652 IH2O 0001 000015 IMAT 0001 003713 INJPS 0001 003713 INJPS
0001 003040 IOFUEL 0001 001746 IOPT 0001 001760 IOU 0001 003242 IOXID 0001 002727 IPROX 0001 002727 IPROX
0001 000016 IQ1 0001 000005 ISV 0001 001626 IUSE 0001 001757 J 0001 001761 JJ 0001 001761 JJ
0001 001613 JOPT 0001 000001 JOU 0001 000014 KMAT 0001 001763 KOUT 0001 000012 L 0001 000012 L
0001 000000 LINE1 0001 001767 LL 0001 001769 LN 0001 001765 LI 0001 001765 LI 0001 001765 LI
0001 000006 MOLES 0001 001772 N 0001 000007 NAME 0001 001754 NASH 0001 001753 NCAL 0001 001753 NCAL
0001 001747 NDUMMY 0001 001755 NFUEL 0001 001762 NI 0001 000017 NOF 0001 000020 NOHIT 0001 000020 NOHIT
0001 000010 NT 0001 000007 NP 0001 000011 NPT 0001 001745 NREAC 0001 000013 NS 0001 000013 NS
0001 001365 PECVT 0001 000304 OFUEL 0001 001015 OMIT 0001 001751 OTEMP 0001 003242 OXID 0001 003242 OXID
0001 001632 RMOL 0001 000003 PER 0001 002727 PROX 0001 002002 PX 0001 000000 RDYES 0001 000000 RDYES
0001 000004 SP 0001 001500 RTEMP 0001 000406 S 0001 001770 SINRT 0001 001660 SLN 0001 001660 SLN
0001 002004 SUM3 0001 015364 SUB 0001 001771 SUM 0001 001773 SUM1 0001 001775 SUM2
0001 002004 SUM3 0001 016514 TEMP 0001 000002 TP 0001 000002 MCR 0001 000002 MCR

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00101 1* SUBROUTINE COALCV(FIRST)
00101 2* USE MIPS INPUT ROUTINES TO READ COAL CONVERSION
00101 3* AND CREATE SIMULATED REACTANT CARDS
00103 4* COMMON /CFUEL/CF,HHVV,WCR,PER
00104 5* COMMON /SPECES/COEF(2,7,150),S(150),EMLN(150),HO(150)
00104 6* X DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150)
00105 7* COMMON /INDEX/IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,NP,NT,NPT,L,NS,
00105 8* X KMAT,IMAT,IQ1,NOF,NOHIT
00106 9* COMMON /CCC/GRAPH,JOUT,DEMAND
00106 10* INTEGER OMIT
00107 11* DIMENSION OMIT(3,50)
00110 12* EQUIVALENCE (OMIT(1,1),ENLN(1))
00111 13* LOGICAL FIRST,RDYES
00111 14* DIMENSION LINE(17)

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OF POOR QUALITY

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00114 15* DATA LINE1/42H TYPE YES TO READ IN PREVIOUS COMPOSITION /
00114 16* DATA ARRAYS FOR REACTANT CARDS
00116 17* DIMENSION NAME(15,25), ANUM(15,25), PECUT(25), MOLE(25), FETH(25),
00116 18* X FAZ(25), PTMP(25), FOX(25), DENS(25)
00117 19* DIMENSION IFAZ(15)
00120 20* EQUIVALENCE (FAZ(1),IFAZ(1))
00120 21* ARRAYS FOR COAL DATA
00120 22* DIMENSION IPROX(3)
00122 23* DIMENSION PROX(3), COAL(5,2), ICCOMP(12,5), ICCOMP(12,5),
00122 24* X OFUEL(13,10), IOFUEL(13,10), OXID(11,5), IOXID(11,5),
00122 25* X ACOMP(11,8), IACOMP(11,8)
00123 26* EQUIVALENCE (PROX(1),IPROX(1))
00124 27* EQUIVALENCE (COAL(1,1),ICOAL(1,1))
00125 28* EQUIVALENCE (ICOMP(1,1),ICCOMP(1,1))
00126 29* EQUIVALENCE (OFUEL(1,1),IOFUEL(1,1))
00127 30* EQUIVALENCE (OXID(1,1),IOXID(1,1))
00130 31* EQUIVALENCE (ACOMP(1,1),IACOMP(1,1))
00131 32* DIMENSION JOPT(10)
00132 33* DIMENSION ID(5), RMOL(5)
00133 34* DATA (ID(1),1,1,5)/C, 'H', 'N', 'O', 'S' /
00135 35* DATA (RMOL(1),1,1,5)/12.0115,1.00797,14.0067,15.994,32.064/
00137 36* DIMENSION ASH(10,5), IASH(10,5)
00140 37* EQUIVALENCE (ASH(1,1),IASH(1,1))
00141 38* DATA (IASH(1,1),1,1,10,2)/SI, 'O', '3' /
00143 39* DATA (IASH(1,2),1,1,10,2)/FE, 'O', '3' /
00145 40* DATA (IASH(1,3),1,1,10,2)/AL, 'O', '3' /
00147 41* DATA (IASH(1,4),1,1,10,2)/FE, 'S', '3' /
00151 42* DATA (ASH(1,1),1,2,10,2)/1,2,3,0./
00153 43* DATA (ASH(1,2),1,2,10,2)/2,3,3,0./
00155 44* DATA (ASH(1,3),1,2,10,2)/2,3,3,0./
00157 45* DATA (ASH(1,4),1,2,10,2)/1,2,3,0./
00161 46* DIMENSION CC(5), ICC(5)
00162 47* DATA (ICC(1),1,1,5)/C, '4', '4' /
00164 48* DATA (CC(1),1,1,5)/1,4,4,0./
00166 49* DIMENSION IH2O(5), H2O(5)
00167 50* DATA (IH2O(1),1,1,5)/H, 'O', '3' /
00171 51* DATA (H2O(1),1,1,5)/2,1,3,0./
00173 52* DIMENSION HHT(40), HH(4)
00174 53* DATA (HHT(1),1,1,40)/
00174 54* X 0 - E, 'INTER D', 'ATA', '2' /
00174 55* X 1 - D, 'ULONG', '1', '2' /
00174 56* X 2 - D, 'ULONG', '2', '2' /
00174 57* X 3 - C, 'PP2', '3' /
00174 58* X 4 - 6, 'RUMEL', 'DAVIS', '2' /
00174 59* X 5 - C, 'CSTOB', '3' /
00174 60* X 6 - M, 'AX OF', 'ABOVE', '2' /
00174 61* X 7 - M, 'IN OF', 'ABOVE', '2' /
00174 62* X /
00176 63* DATA IC/12/
00176 64* CALL PAGIT
00201 65* CALL CHR$IZ(4)
00202 66* NREAC=0
00203 67* IOPT=0
00204 68* DO 2 I=1,10
00207 69* 2 JOPT(I)=1
00211 70* DO 12 I=1,5

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00214 71* 12 ICOAL(I,1)=ID(I) 000016
00215 72* C FOR FIRST PASS DO NOT CHECK SAVED DATA 000016
00216 73* IF (.NOT.FIRST) GO TO 10 000020
00220 74* IF (.NOT.RDYES(LINE1,92)) GO TO 300 000022
00222 75* 10 CONTINUE 000030
00222 76* C READ IN PREVIOUS COAL DATA 000030
00223 77* RFWIND IC 000030
00224 78* READ (IC) NDMY,CF,HVV,MCR,PER 000032
00224 79* READ (IC) CTMP,OTEMP 000043
00237 80* READ (IC) PROX,COAL,PER,IE,HH 000051
00246 81* READ (IC) NCOAL,NASH,MFUEL,NOXID 000071
00254 82* READ (IC) ICOMP(J),I=1,12,J=1,MCOALJ, 000112
00254 83* X ICOMP(J),I=1,12,J=1,MASHJ, 000112
00254 84* X ICOMP(J),I=1,12,J=1,MFUELJ, 000112
00254 85* X ICOMP(J),I=1,12,J=1,MNOXIDJ, 000112
00254 86* C DISPLAY PRESENT COAL DATA 000112
00312 87* IF (FIRST) GO TO 50 000150
00314 88* IF (.NOT.RDYES(LINE1,92)) GO TO 300 000152
00316 89* 50 CONTINUE 000160
00317 90* CALL GOUT(' 1 - VOLATILE (OPTIONAL) AND ASH AS LBS/100 LBS DRY COA 000160
00317 91* XL',56) 000160
00320 92* ENCODE (56,IOUT) PROX(1) 000163
00323 93* 56 FORMAT (6X,'VOLATILE',F10.4) 000171
00324 94* CALL GOUT(IOUT,24) 000171
00325 95* ENCODE (56,IOUT) PROX(3) 000175
00330 96* 58 FORMAT (6X,'ASH',5X,F10.4) 000203
00331 97* CALL GOUT(IOUT,24) 000207
00332 98* CALL GOUT(' 1) 000213
00333 99* ENCODE (60,IOUT) CTMP 000221
00336 100* 60 FORMAT (' 2 - COAL TEMPERATURE IN DEG F',F10.2) 000221
00337 101* CALL GOUT(IOUT,40) 000221
00340 102* CALL GOUT(' 1) 000225
00341 103* CALL GOUT(' 3 - DRY COAL COMPOSITION AS LBS/100 LBS DRY COAL',49) 000231
00342 104* DO 66 I=1,5 000240
00345 105* ENCODE (62,IOUT) ICOAL(I,1),COAL(I,2) 000240
00351 106* 62 FORMAT (5X,A5,F10.4) 000246
00352 107* CALL GOUT(IOUT,24) 000246
00353 108* 66 CONTINUE 000253
00355 109* CALL GOUT(' 1) 000253
00356 110* CALL GOUT(' 4 - OTHER COAL COMPONENTS AS LBS/100 LBS DRY COAL, 51A 000257
00356 111* XTE AND COMPOSITION',73) 000257
00357 112* IF (NCOAL.EQ.0) GO TO 80 000263
00361 113* DO 72 I=1,NCOAL 000265
00364 114* ENCODE (70,IOUT) CCOMP(I,1),ICOMP(2,1), 000273
00364 115* X ICOMP(J*2+1,1),CCOMP(J*2+2,1),J=1,5) 000273
00375 116* 70 FORMAT (F10.4,10X,A5,5(2X,A2,2X,F8.4)) 000306
00376 117* CALL GOUT(IOUT,94) 000306
00377 118* 72 CONTINUE 000316
00401 119* 80 CALL GOUT(' 1) 000316
00402 120* CALL GOUT(' 5 - ASH COMPOSITION AS LBS/100 LBS ASH AND COMPONENT', 000321
00402 121* X 53) 000321
00403 122* IF (NASH.EQ.0) GO TO 90 000325
00405 123* DO 84 I=1,NASH 000327
00410 124* ENCODE (84,IOUT) ACOMP(I,1),IACOMP(J*2+1,1),J=1,5) 000335
00420 125* 84 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4)) 000347
00421 126* CALL GOUT(IOUT,94) 000347

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COALCV

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00422 127* 8A CONTINUE 000357
00424 128* 9D CALL GOUT(' ',1) 000357
00425 129* ENCODE (92,100) PER 000362
00430 130* 92 FORMAT (1, ' - FRACTION CARBON CONVERSION',F10.4) 000370
00431 131* CALL GOUT(100,41) 000370
00432 132* CALL GOUT(' ',1) 000374
00433 133* ENCODE (96,100) HHEI(1) 000400
00434 134* 96 FORMAT (1, 7 - HEATING VALUE OF COAL BTU/LB*,F13.3) 000410
00435 135* CALL GOUT(100,46) 000410
00440 136* CALL GOUT(' ',1) 000414
00441 137* CALL GOUT(' 8 - OTHER FUEL COMPONENTS AS LBS/LB COAL, TEMPERATURE 000420
00441 138* XIN DEG F, STATE AND COMPOSITION',86) 000420
00442 139* IF (FUEL.EQ.0) GO TO 104 000424
00444 140* DO 102 I=1,NFUEL 000426
00447 141* ENCODE (100,100) OFUEL(1,1),OFUEL(2,1),OFUEL(3,1), 000434
00447 142* X (10,FUEL(1,2,2,1),OFUEL(J+2,3,1),J=1,5) 000434
00461 143* 100 FORMAT (F10.4,F10.3,1X,A3,5(2X,A2,2X,F8.4)) 000450
00462 144* CALL GOUT(100,94) 000450
00463 145* 102 CONTINUE 000460
00465 146* 104 CALL GOUT(' ',1) 000460
00466 147* ENCODE (106,100) OTEMP 000763
00471 148* 106 FORMAT (1, 9 - OXIDIZER TEMPERATURE IN DEG F*,F10.2) 000771
00472 149* CALL GOUT(100,94) 000771
00473 150* CALL GOUT(' ',1) 000775
00474 151* CALL GOUT(' 10 - OXIDIZER COMPONENTS AS LBS/100 LBS OXIDIZER AND C 000501
00474 152* X COMPONENT',63) 000501
00475 153* IF (NOXID.EQ.0) GO TO 112 000505
00477 154* DO 110 I=1,NOXID 000507
00502 155* ENCODE (108,100) OXID(1,1),OXID(J+2,1),OXID(J+2,1,1),J=1,5) 000515
00512 156* 108 FORMAT (F10.4,14X,5(2X,A2,2X,F8.4)) 000527
00513 157* CALL GOUT(100,94) 000527
00514 158* 110 CONTINUE 000537
00516 159* 112 CALL GOUT(' ',1) 000537
00517 160* CALL GOUT(' TYPE 1 OR 2 TO MODIFY OR REPLACE',33) 000542
00520 161* CALL GOUT(' RETURN TO CONTINUE',23) 000546
00521 162* IOPT=0 000552
00522 163* 114 CONTINUE 000554
00523 164* CALL ROATAT(1,IOPT,514) 000554
00524 165* IF (IOPT.LT.0.OR.IOPT.GT.2) GO TO 114 000560
00526 166* IF (IOPT.EQ.0) GO TO 680 000575
00530 167* GO TO (120,300),IOPT 000577
00530 168* C SELECT GROUPS TO BE CHANGED 000577
00531 169* 120 CONTINUE 000611
00532 170* DO 124 I=1,10 000611
00535 171* 124 JOPT(I)=0 000611
00537 172* CALL GOUT(' TYPE GROUP NUMBERS OF DATA TO BE CHANGED IN ASCENDING 000612
00537 173* X ORDER, FOR EXAMPLE 1 3 7 9',83) 000612
00540 174* 126 CONTINUE 000617
00541 175* CALL ROATAT(10,JOPT,5126) 000617
00542 176* DO 130 I=10,1,-1 000626
00545 177* JJ=JOPT(I) 000626
00546 178* IF (JJ.EQ.0) GO TO 130 000627
00550 179* JOPT(I)=0 000631
00551 180* JOPT(JJ)=JJ 000633
00552 181* 130 CONTINUE 000637
00552 182* C ADD OR UPDATE COAL DATA 000637

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COALCV

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00554 103* 300 CONTINUE
00555 180* CALL PAGIT
00556 185* IF (JOPT(1).EQ.0) GO TO 314
00557 186* READ IN PROXIMATE ANALYSIS DATA
00558 187* C 310 CALL GOUT(' TYPE (OPTIONAL) LBS VOLATILES/100 LBS DRY COAL',*71)
00559 188* CALL RDATAF(1,PROX(1),*310)
00560 189* IF (IPROX(1).EQ.* ) PROX(1)=0.
00561 190* 312 CALL GOUT(' TYPE LBS ASH/100 LBS DRY COAL',*30)
00562 191* CALL RDATAF(1,PROX(3),*312)
00563 192* PROX(2)=100.-PROX(1)-PROX(3)
00564 193* 314 IF (JOPT(2).EQ.0) GO TO 320
00565 194* C READ IN COAL TEMPERATURE
00566 195* 316 CALL GOUT(' TYPE COAL TEMPERATURE IN DEG F',*31)
00567 196* CALL RDATAF(1,CTEMP,*316)
00568 197* 320 IF (JOPT(3).EQ.0) GO TO 340
00569 198* C READ IN REACTING COAL COMPOSITION
00570 199* CALL GOUT(' TYPE LBS/100 LBS DRY COAL FOR ELEMENTS',*39)
00571 200* 322 CALL GOUT(' C',*2)
00572 201* CALL RDATAF(1,COAL(1),*2),*322)
00573 202* 324 CALL GOUT(' H',*2)
00574 203* CALL RDATAF(1,COAL(2),*324)
00575 204* 326 CALL GOUT(' N',*2)
00576 205* CALL RDATAF(1,COAL(3),*2),*326)
00577 206* 328 CALL GOUT(' O',*2)
00578 207* CALL RDATAF(1,COAL(4),*2),*328)
00579 208* 330 CALL GOUT(' S',*2)
00580 209* CALL RDATAF(1,COAL(5),*2),*330)
00581 210* 340 IF (JOPT(4).EQ.0) GO TO 350
00582 211* C READ IN OTHER COAL COMPONENTS
00583 212* CALL GOUT(' TYPE (OPTIONAL) OTHER COAL COMPONENTS',*38)
00584 213* CALL GOUT(' TYPE LBS/100 LBS DRY COAL, STATE AND COMPONENT',*50)
00585 214* CALL GOUT(' COAL TEMPERATURE IS ASSUMED',*28)
00586 215* NI=1
00587 216* 342 CALL GOUT(' EXAMPLE 0.13 1HG 2HCL 2',*32)
00588 217* 343 DO 344 J=1,5
00589 218* ICCOMP(J*2+1,NI)=2H
00590 219* CCOMP(J*2+2,NI)=0.
00591 220* 344 CCOMP(1,NI)=0.
00592 221* ICCOMP(2,NI)=*
00593 222* 346 CALL RDATAF(12,CCOMP(1,NI),*342)
00594 223* IF (ICOMP(1,NI)) *344
00595 224* IF (ICOMP(1,NI).EQ.* ) GO TO 348
00596 225* NI=NI+1
00597 226* GO TO 343
00598 227* 348 NCOAL=NI-1
00599 228* 350 IF (JOPT(5).EQ.0) GO TO 380
00600 229* IF (JOPT(NE.1)) GO TO 351
00601 230* ENCODE (2350,1OUT) JOPT(5)
00602 231* 2350 FORMAT (' GROUP NUMBER',15)
00603 232* CALL GOUT(1OUT,18)
00604 233* 2352 IF (WASH.EQ.0) GO TO 2357
00605 234* DO 2354 I=1,NASH
00606 235* ENCODE (2354,1OUT) I,ACOMP(1,I)
00607 236* IF (ACOMP(J*2+1,I)) I,ACOMP(J*2+1,I),J=1,5
00608 237* X FORMAT (14,F10.4,14X,5(2X,A2,2X,FR.4))
00609 238* 2354 CALL GOUT(1OUT,98)
00610 239*
00611 240*
00612 241*
00613 242*
00614 243*
00615 244*
00616 245*
00617 246*
00618 247*
00619 248*
00620 249*
00621 250*
00622 251*
00623 252*
00624 253*
00625 254*
00626 255*
00627 256*
00628 257*
00629 258*
00630 259*
00631 260*
00632 261*
00633 262*
00634 263*
00635 264*
00636 265*
00637 266*
00638 267*
00639 268*
00640 269*
00641 270*
00642 271*
00643 272*
00644 273*
00645 274*
00646 275*
00647 276*
00648 277*
00649 278*
00650 279*
00651 280*
00652 281*
00653 282*
00654 283*
00655 284*
00656 285*
00657 286*
00658 287*
00659 288*
00660 289*
00661 290*
00662 291*
00663 292*
00664 293*
00665 294*
00666 295*
00667 296*
00668 297*
00669 298*
00670 299*

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00671 239* 2356 CONTINUE 001137
00673 240* 2357 CALL GOUT1 TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE*,503 001137
00674 241* 2358 KOUT=0 001143
00675 242* 001150
00676 243* 001165
00700 244* 001167
00702 245* 001172
00704 246* 001177
00705 247* 001177
00706 248* 001204
00707 249* 001221
00711 251* 001221
00713 252* 001224
00714 253* 001227
00716 254* 001234
00721 255* 001245
00724 256* 001245
00725 257* 001250
00730 258* 001250
00731 259* 001252
00731 260* 001252
00732 261* 001254
00733 262* 001255
00733 263* 001255
00734 264* 001257
00735 265* 001261
00735 266* 001261
00736 267* 001263
00737 268* 001266
00742 269* 001300
00743 270* 001301
00745 271* 001303
00746 272* 001313
00746 273* 001313
00747 274* 001315
00750 275* 001315
00753 276* 001334
00756 277* 001334
00760 278* 001337
00762 279* 001346
00764 280* 001346
00765 281* 001350
00766 282* 001354
00770 283* 001354
00771 284* 001356
00771 285* 001356
00772 286* 001356
00773 287* 001361
00774 288* 001366
00775 289* 001371
00776 290* 001377
00777 291* 001402
01000 292* 001410
01001 293* 001411
01002 294* 001421

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2356 CONTINUE

2357 CALL GOUT1 TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE*,503

2358 KOUT=0

CALL RDATA1(I,KOUT,52358)

IF (KOUT.LT.0.OR.KOUT.GT.3) GO TO 2358

IF (KOUT.EQ.0) GO TO 2380

IF (KOUT.EQ.3) GO TO 2370

CALL GOUT1 TYPE LINE NUMBER*,17)

2360 LN=0

CALL RDATA1(I,LN,52360)

IF (LN.LE.0.OR.LN.GT.NASH) GO TO 2360

IF (KOUT.EQ.1) GO TO 2366

DELETE

LI=LN

IF (LN.EQ.NASH) GO TO 2364

DO 2362 I=LI,NASH

DO 2362 J=1,11

ACOMP(J,I-1)=ACOMP(J,I)

CONTINUE

2362 NASH=NASH-1

2364 NASH=NASH-1

GO TO 2352

C

2366 NI=LN

GO TO 2372

C

ADD

2370 NASH=NASH+1

NI=NASH

C

READ IN NEW DATA

2372 CALL GOUT1 LBS/100 LBS DRY ASH AND COMPONENT*,34)

DO 2374 J=1,5

IACOMP(J,2,NI)=2H

2374 IACOMP(J,2,NI)=0

CALL RDATA1(I,ACOMP(I,NI),52372)

GO TO 2352

C

CHECK FOR FES2

2380 FES2=0

DO 2386 I=1,NASH

DO 2386 J=1,5

IF (IACOMP(J,2,I).NE.IASH(J,2-1,N)) GO TO 2386

IF (IACOMP(J,2+1,I).NE.ASH(J,2,N)) GO TO 2386

CONTINUE

2384 FES2=ACOMP(1,1)

GO TO 380

2386 CONTINUE

GO TO 380

351 CONTINUE

C

READ IN ASH COMPONENTS

CALL GOUT1 TYPE LBS/100 LBS DRY ASH FOR COMPONENTS*,40)

CALL GOUT1 STATE ASSUMED SOLID, COAL TEMPERATURE ASSUMED*,47)

352 CALL GOUT1 S102*,5)

CALL RDATA1(I,ACOMP(1,1),5352)

354 CALL GOUT1 FE203*,6)

CALL RDATA1(I,ACOMP(1,2),5354)

356 CALL GOUT1 AL2O3*,6)

CALL RDATA1(I,ACOMP(1,3),5356)

358 CALL GOUT1 FES2*,5)

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01001 295*      CALL RDATAF(1,ACOMP(1,4),3350)      001424
01002 296*      PES2=ACOMP(1,4)                    001431
01003 297*      IF (IACOMP(1,4).EQ.0) FES2=0.      001433
01004 298*      J=0                                  001437
01005 299*      REMOVE ANY ZERO COMPONENTS          001437
01006 300*      DO 364 I=1,N                          001444
01007 301*      IF (IACOMP(1,I).NE.0)              001450
01008 302*      IF (IACOMP(1,I).EQ.0)              001452
01009 303*      J=J+1                                001455
01010 304*      ACOMP(1,J)=ACOMP(1,I)              001461
01011 305*      IF (I.NE.J) ACOMP(1,I)=0.          001462
01012 306*      DO 362 LL=1,10                      001466
01013 307*      362 ACOMP(LL+1,J)=ASHILL(I)         001477
01014 308*      364 CONTINUE                        001504
01015 309*      NI=J+1                              001504
01016 310*      C ADD OTHER ASH COMPONENTS          001504
01017 311*      CALL GOUT(' CONTINUE WITH ASH COMPONENTS',29) 001507
01018 312*      CALL GOUT(' LBS/100 LBS DRY ASH AND COMPONENT',29) 001513
01019 313*      366 CALL GOUT(' EXAMPLE 0.25 2HTI 1. 1HO 2.,3A) 001520
01020 314*      367 DO 368 J=1,N                    001524
01021 315*      IACOMP(J+2,NI)=2H                  001535
01022 316*      368 ACOMP(J+2+1,NI)=0.              001536
01023 317*      370 CALL RDATAF(1,ACOMP(1,NI),3366) 001540
01024 318*      IF (IACOMP(1,NI)) 372,            001550
01025 319*      IF (IACOMP(1,NI).EQ.0)            001552
01026 320*      NI=NI+1                             001555
01027 321*      GO TO 367                           001560
01028 322*      372 NASH=NI-1                       001562
01029 323*      380 IF (JOPT(4).EQ.0) GO TO 390      001565
01030 324*      C READ COAL CONVERSION FRACTION      001565
01031 325*      382 CALL GOUT(' TYPE CARBON CONVERSION FRACTION, FOR EXAMPLE, 0.89', 001567
01032 326*      X 51)                                001567
01033 327*      C CALL RDATAF(1,PER,3382)            001572
01034 328*      COMPUTE VALUES FOR HHV BY DIFFERENT FORMULAS 001572
01035 329*      390 CONTINUE                          001600
01036 330*      HH(2)=185.89*COAL(1,2)+620.28*(COAL(2,2)-0.125*COAL(N,2)) 001600
01037 331*      X +40.50*COAL(5,2)                  001600
01038 332*      HH(3)=186.0*COAL(1,2)+620.0*(COAL(2,2)-0.125*COAL(N,2)) 001614
01039 333*      X +40.50*COAL(5,2)                  001614
01040 334*      HH(4)=184.9*COAL(1,2)+610.0*(COAL(2,2)-0.125*COAL(N,2)) 001623
01041 335*      X +55.50*COAL(5,2)                  001623
01042 336*      HH(5)=(658.3*COAL(2,2)/(100.-PROX(3))+24.62)* 001634
01043 337*      X (COAL(1,2)/3.+COAL(2,2)-0.125*(COAL(N,2)-COAL(5,2))) 001634
01044 338*      HH(6)=146.58*COAL(1,2)+568.78*COAL(2,2)+29.4*COAL(5,2) 001653
01045 339*      X -6.58*PROX(3)-51.53*(COAL(3,2)+COAL(N,2)) 001653
01046 340*      HH(7)=AMX1*HH(2)+HH(3),HH(4),HH(5),HH(6)) 001673
01047 341*      HH(8)=AMIN1*HH(2),HH(3),HH(4),HH(5),HH(6)) 001715
01048 342*      DO 392 I=2,N                          001743
01049 343*      ENCODE (394,HH(I+5-1)) HH(I)        001743
01050 344*      392 CONTINUE                          001753
01051 345*      394 FORMAT (F12.3)                  001753
01052 346*      IF (JOPT(7).EQ.0) GO TO 420          001753
01053 347*      CALL GOUT(' HHV CALCULATION',16)      001755
01054 348*      DO 394 I=1,8                          001764
01055 349*      CALL GOUT(' I=5-8',30)              001764
01056 350*      398 CONTINUE                        001771

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01114 331* 400 CALL RDATA1(1,12,5400)
01115 352* IF (IE.LI-D.04-IE-G.8) GO TO 400
01117 353* IF (IE.RI-D) GO TO 420
01121 354* 402 CALL GOUT1* ENTER HWY AS BTU/LB COAL*,25)
01123 355* CALL RDATA1(1,HH(1),5402)
01124 356* 420 HWY=HH(1)+1)
01126 357* IF (JOPT(1),EQ.0) GO TO 440
01128 358* IF (IOPT(NE.1) GO TO 421
01130 359* ENCODE 12350,IOUT, JOP(18)
01133 360* CALL GOUT1(1,OUT,18)
01134 361* 2420 IF (IN.4-EO.0) GO TO 2427
01136 362* DO 2426 1-1,NFUEL
01141 363* ENCODE 12428,IOUT) 1,OFUEL(1,1),OFUEL(12,1),OFUEL(13,1),
01141 364* X (OFUEL(J*2+2,1),OFUEL(J*2,1),J=1,5)
01154 365* 2428 FORMAT (19,F10.9,F10.3,1X,A3,5I2X,A2,2X,E6.4)
01155 366* CALL GOUT1(OUT,98)
01156 367* 2426 CONTINUE
01160 368* 2427 CALL GOUT1* TYPE 1-ALTER, 2-DELETE, 3-ADD, RETURN TO CONTINUE*,50)
01161 369* 2422 KOUT=0
01162 370* CALL RDATA1(1,KOUT,52422)
01163 371* IF (KOUT-LT-D.08-KOUT-GT.3) GO TO 2422
01165 372* IF (KOUT-EQ.0) GO TO 430
01167 373* IF (KOUT-EQ.3) GO TO 2434
01171 374* CALL GOUT1* TYPE LINE NUMBER*,17)
01172 375* 2428 LN=0
01173 376* CALL RDATA1(1,LN,52428)
01174 377* IF (LN-LT-D.08-LN-GT,NFUEL) GO TO 2428
01176 378* IF (KOUT-EQ.1) GO TO 2432
01176 379* C DELETE
01200 380* LI=LN+1
01201 381* IF (LN-EQ,NFUEL) GO TO 2431
01203 382* DO 2430 1-1,NFUEL
01206 383* DO 2430 J=1,13
01211 384* OFUEL(J,1)=OFUEL(J,1)
01212 385* 2430 CONTINUE
01215 386* 2431 NFUEL=NFUEL-1
01216 387* GO TO 2420
01216 388* C ALTER
01217 389* 2432 NI=LN
01220 390* C AND GO TO 2436
01220 391* 2434 NFUEL=NFUEL+1
01221 392* NI=NFUEL
01222 393* C READ IN NEW DATA
01222 394* 2436 CALL GOUT1* TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO
01223 395* COMPONENT*,63)
01223 396* DO 2438 1-1,5
01224 397* 2438 OFUEL(J*2+2,NI)=2H
01227 398* OFUEL(J*2+3,NI)=0.
01230 399* OFUEL(1,NI)=0.
01232 400* OFUEL(2,NI)=0.
01233 401* OFUEL(3,NI)=0.
01234 402* OFUEL(13,NI)=0.
01235 403* CALL RDATA1(1,OFUEL(1,NI),52436)
01236 404* GO TO 2420
01237 405* 421 CONTINUE
01237 406* C READ IN OTHER FUEL COMPONENTS

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01240 907* CAL GOUT(' TYPE OTHER FUEL COMPONENTS',27)
01241 908* CALL GOUT(' TYPE LBS/LB COAL, TEMPERATURE (DEG F) AND STATE AND CO
01242 909* COMPONENT',63)
01243 910* NI=1
01244 911* 422 CALL GOUT(' EXAMPLE 0.31 100. 1HG 1HH 2. 1HO 1.,47)
01245 912* 423 DO 424 J=1,5
01246 913* 10FUEL(J*2+2,NI)=2H
01247 914* 10FUEL(J*2+3,NI)=0.
01248 915* 10FUEL(1,NI)=0.
01249 916* 10FUEL(2,NI)=0.
01250 917* 10FUEL(3,NI)=0.
01251 918* 426 CALL RDATAF(13,10FUEL(1,NI),422)
01252 919* IF (10FUEL(1,NI) .NE. 1H20) * ) GO TO 428
01253 920* IF (10FUEL(1,NI) .EQ. 0) * ) GO TO 428
01254 921* NI=NI+1
01255 922* GO TO 423
01256 923* 428 MFUEL=NI-1
01257 924* 430 WCR=0.
01258 925* DO 434 I=1,MFUEL
01259 926* DO 432 J=1,5
01260 927* IF (10FUEL(J*2+2,I).NE.1H20(J)) GO TO 434
01261 928* IF (10FUEL(J*2+3,I).NE.1H20(J)) GO TO 434
01262 929* 432 CONTINUE
01263 930* WCR=0FUEL(1,I)
01264 931* GO TO 440
01265 932* 434 CONTINUE
01266 933* 440 IF (JOPT(9).EQ.0) GO TO 450
01267 934* READ IN OXIDIZER TEMPERATURE
01268 935* 442 CALL GOUT(' TYPE IN OXIDIZER TEMPERATURE, DEG F',36)
01269 936* CALL RDATAF(1,OTEMP,442)
01270 937* 450 IF (JOPT(10).EQ.0) GO TO 470
01271 938* READ IN OXIDIZER COMPONENTS
01272 939* CALL GOUT(' TYPE OXIDIZER COMPONENTS',25)
01273 940* CALL 5OUT(' TYPE LBS/100 LBS OXIDIZER AND COMPONENT',40)
01274 941* NI=1
01275 942* 452 CALL GOUT(' EXAMPLE 95.0 1HO 2.,27)
01276 943* 453 DO 454 J=1,5
01277 944* 10OXID(J*2,NI)=2H
01278 945* 454 OXID(J*2+1,NI)=0.
01279 946* 456 CALL RDATAF(11,OXID(1,NI),452)
01280 947* IF (OXID(1,NI) .EQ. 0) * ) GO TO 460
01281 948* IF (OXID(1,NI) .EQ. 0) * ) GO TO 460
01282 949* NI=NI+1
01283 950* GO TO 453
01284 951* 460 NOXID=NI-1
01285 952* 470 CONTINUE
01286 953* C COMPUTATION FOR COAL CARD
01287 954* SIMPL=COAL(1,2)*(1.-PER)
01288 955* COAL(1,2)=COAL(1,2)*PER
01289 956* SUM=0.
01290 957* M=NKAC*1
01291 958* MS=N
01292 959* 482 I=1,5
01293 960* 482 S M=SUM+COAL(I,2)
01294 961* DO 484 I=1,5
01295 962* 484 AUMEN,I)=(COAL(I,2)/SUM)*100.
01296 963*

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01360 463* SUM=0.
01361 464* DO 466 I=1,5
01364 465* ANUMIN,I)=ANUMIN,I)/PMOL,I)
01365 466* 486 SUM=SUM1+ANUMIN,I)
01367 467* DO 468 I=1,5
01372 468* 488 ANUMIN,I)=ANUMIN,I)/SUM1*100.
01372 469* C CREATE COAL CARD
01374 470* DO 494 I=1,5
01377 471* 494 NAMEIN,I)=ICOL(I,1)
01401 472* NAMEIN,6)=H
01402 473* ANUMIN,6)=0.
01402 474* C COMPUTE COAL/FUEL RATIO
01403 475* CSUM=0.
01404 476* DO 498 I=1,NFUEL
01407 477* 498 CSUM=CSUM+OFUEL(I,1)
01411 478* CF=1.0/(1.0+CSUM)
01413 479* PECWTIN)=CF*SUM/100.
01413 480* MOLEIN)=H
01414 481* FAZIN)=1H5
01415 482* RTMPIN)=(TEMP-32.1)/1.8*273.15
01416 483* FOXIN)=1HF
01417 484* DENSIN)=0.
01420 485* NREAC=NREAC+1
01420 486* C CREATE INERT CARBON CARD
01421 487* IF (PER-1.) .504,
01424 488* N=NREAC+1
01425 489* DO 500 I=1,6
01430 490* NAMEIN,I)=H
01431 491* ANUMIN,2)=0.
01433 492* ANUMIN,I)=1C
01434 493* ANUMIN,1)=1.
01435 494* PECWTIN)=CF*SINRT/100.
01436 495* MOLEIN)=H
01437 496* ENTHIN)=0.
01440 497* NAMEIN,6)=2H00
01441 498* FAZIN)=1H5
01442 499* RTMPIN)=RTMPIN(S)
01443 500* FOXIN)=1HF
01444 501* DENSIN)=0.
01445 502* NREAC=NREAC+1
01445 503* C CREATE OTHER COAL COMPONENTS CARDS
01446 504* 504 IF (NCOAL.EQ.0) GO TO 520
01450 505* N=NREAC
01451 506* DO 508 I=1,NCOAL
01454 507* DO 506 J=1,5
01457 508* NAMEIN,I,J)=ICCOMP(J*2+1,I)
01460 509* ANUMIN,I,J)=CCOMP(J*2+2,I)
01462 510* PECWTIN,I)=CCOMP(I,1)*CF/100.
01463 511* MOLEIN,I)=H
01464 512* IF (FAZIN,I)=ICCOMP(12,I)
01465 513* ENTHIN,I)=0.
01466 514* NAMEIN,I,6)=2H00
01467 515* ANUMIN,I,6)=0.
01470 516* RTMPIN,I)=TEMP-32.1/1.8*273.15
01471 517* FOXIN,I)=1HF
01472 518* DENSIN,I)=0.

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01473 519* 508 CONTINUE
01475 520* 520 NREAC=NREAC+NCOAL
01475 521* C CREATE CARDS FOR ASH COMPONENTS
01476 522* N=NREAC
01477 523* SUM2=0
01500 524* IF (NASH.EQ.0) GO TO 540
01500 525* ASHF=CF*PROX(3)/100.
01503 526* DO 522 I=1,NASH
01506 527* 522 SUM2=SUM2+ACOMP(I,I)
01510 528* DO 528 I=1,NASH
01513 529* DO 526 J=1,5
01516 530* NAME(N+I,J)=IACOMP(J*2,I)
01517 531* 526 ANUM(N+I,J)=ACOMP(J*2,I,I)
01521 532* PECWT(N+I)=ACOMP(1,I)*ASHF)/SUM2
01522 533* MOLE(N+I)=1H
01523 534* FAZ(N+I)=1HS
01524 535* ENTH(N+I)=0.
01525 536* NAME(N+1,61)=2H00
01526 537* ANUM(N+1,61)=0.
01527 538* RTEMP(N+1)=(CTEMP-32.)/1.8+273.15
01530 539* FOX(N+1)=1HF
01531 540* DENS(N+1)=0.
01532 541* 528 CONTINUE
01534 542* 540 NREAC=NREAC+NASH
01534 543* C COMPUTE ENTHALPY FOR COAL
01535 544* FES2=FES2+ASHF/(SUM2*CF)
01536 545* HHV=(1HHV-14485.7*SIWRT/100.)/1.8*(100./SUM1)+(100./SUM1)*100.
01537 546* FES2C=(100.)/(1.8*119.95)*(100./SUM1)+(100./SUM1)*FES2
01540 547* HF1=-ANUM(NS,1)*94051.8-0.5*ANUM(NS,2)*68317.4
01541 548* X -ANUM(NS,5)*70960.-FES2C*197650.
01541 549* PX=100.*PROX(1)/(PROX(1)+PROX(2))
01542 550* HF2=(1.175*(CTEMP-77)+.0029*PX*(CTEMP-77)+
01542 551* X 0.00025*(CTEMP-60)*2-0.07225)*(100./SUM1)+(100./1.8)
01543 552* ENTH(NS)=HHV+HF1*HF2
01543 553* C CREATE CARDS FOR OTHER FUEL COMPONENTS
01544 554* N=NREAC
01545 555* IF (NFUEL.EQ.0) GO TO 560
01547 556* DO 548 I=1,NFUEL
01552 557* DO 546 J=1,5
01553 558* NAME(N+I,J)=IOFUEL(J*2+2,I)
01555 559* ANUM(N+I,J)=OFUEL(J*2+3,I)
01556 560* PECWT(N+I)=OFUEL(I,I)*CF
01560 561* MOLE(N+I)=1H
01561 562* IFAZ(N+I)=IOFUEL(3,I)
01563 563* ENTH(N+I)=0.
01564 564* NAME(N+1,61)=2H00
01565 565* ANUM(N+1,61)=0.
01566 566* RTEMP(N+1)=(OFUEL(2,I)-32.)/1.8+273.15
01567 567* FOX(N+I)=1HF
01570 568* DENS(N+I)=0.
01571 569* 548 CONTINUE
01571 570* C LOOK UP CARBON
01573 571* DO 552 I=1,NFUEL
01576 572* DO 550 J=1,5
01601 573* IF (NAME(N+I,J).NE.ICC(J)) GO TO 552
01603 574* IF (ANUM(N+I,J)-CC(J)) 552,552

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01606 575* 550 CONTINUE
01610 576* GO 10 554
01611 577* 552 CONTINUE
01613 578* GO 10 560
01613 579* C CREATE INERT CARBON CARD FOR RECYCLE CARBON
01619 580* 554 DO 556 J=1,6
01617 581* NAME(N,NFUEL,I,J)=NAME(N,I,J)
01620 582* ANUM(N,NFUEL,I,J)=ANUM(N,I,J)
01622 583* NAME(N,NFUEL,I,J)=IC
01623 584* PECWT(N,NFUEL,I,J)=1.-PER*PECWT(N,I)
01624 585* PECWT(N,I)=PER*PECWT(N,I)
01625 586* MOLE(N,NFUEL,I)=MOLE(N,I)
01626 587* FAZ(N,NFUEL,I)=FAZ(N,I)
01627 588* ENTH(N,NFUEL,I)=ENTH(N,I)
01630 589* RTEMP(N,NFUEL,I)=RTEMP(N,I)
01631 590* FOX(N,NFUEL,I)=FOX(N,I)
01632 591* DENS(N,NFUEL,I)=DENS(N,I)
01633 592* NREAC=NREAC,I
01634 593* 560 NREAC=NREAC,NFUEL
01635 594* C CREATE CARDS FOR OXIDIZER COMPONENTS
01635 595* N=NREAC
01636 596* IF (NOXID.EQ.0) GO TO 590
01640 597* SUM3=0.
01641 598* DO 572 I=1,NOXID
01644 599* SUM3=SUM3+OXID(I,I)
01646 600* DO 578 I=1,NOXID
01651 601* DO 576 J=1,5
01654 602* NAME(N,I,J)=IOXID(J+2,I)
01655 603* ANUM(N,I,J)=OXID(J+2,I,I)
01657 604* PECWT(N,I)=OXID(I,I)/SUM3
01660 605* MOLE(N,I)=1H
01661 606* FAZ(N,I)=1HG
01662 607* ENTH(N,I)=0.
01663 608* NAME(N,I,6)=2HOO
01664 609* ANUM(N,I,6)=0.
01665 610* RTEMP(N,I)=(OTEMP-32.)/1.8+273.15
01666 611* FOX(N,I)=1HO
01666 612* DENS(N,I)=0.
01667 613* 578 CONTINUE
01672 614* 590 NREAC=NREAC+NOXID
01672 615* C SAVE COAL DATA
01673 616* COAL(I,2)=COAL(I,2)/PER
01674 617* REWIND IC
01675 618* WRITE (IC) NREAC,CF,HHVV,UCR,PER
01675 619* WRITE (IC) CTEMP,OTEMP
01675 620* WRITE (IC) PROX,COAL,PER,IE,HH
01675 621* WRITE (IC) NCOAL,NASH,NFUEL,NOXID
01675 622* WRITE (IC) ((COMP(I,J),I=1,11),J=1,NCOAL),
X ((COMP(I,J),I=1,11),J=1,NASH),
X ((NFUEL(I,J),I=1,13),J=1,NFUEL),
X ((OXID(I,J),I=1,11),J=1,NOXID)
01725 623* 576 CONTINUE
01725 624* 590 NREAC=NREAC+NOXID
01725 625* C WRITE OUT REACTANT FILE
01725 626* WRITE (IC) NREAC,CF
01725 627* DO 610 I=1,NREAC
01725 628* WRITE (IC) NAME(I,J),ANUM(I,J),J=1,8),PECWT(I),MOLE(I),
01725 629* WRITE (IC) NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)
01772 630* X ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOX(I),DENS(I)

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OF POOR QUALITY

COALCV

02012	631*	610	CONTINUE	003646
02013	632*		ENDFILE IC	003646
02015	633*	680	CONTINUE	003652
02016	634*		RETURN	003652
02017	635*		END	003712

END OF COMPILATION: NO DIAGNOSTICS.

ADG,P CPHS

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#FOR'S CPHS,CPHS
HSA E3 -10/15/80-13:06:13 (11.)

SUBROUTINE CPHS ENTRY POINT 000567

STORAGE USED: CODE(11) 000603; DATA(0) 000160; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 SPECES 017106
0004 MISC 001701
0005 INDX 000041
0006 LONTH 001201
0007 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0010 NWOUS
0011 NI025
0012 ALOG
0013 NI015
0014 NERR33

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000031	10L	0001	000207	1716	0001	000217	1746	0001	000043	20L	0001	000351	2216
0001	000462	254G	0001	000065	30L	0001	000067	31L	0001	000157	32L	0000	000041	333F
0001	000164	40L	0001	000176	60L	0001	000230	70L	0001	000233	80L	0001	000412	87L
0000	000060	88F	0001	000472	89L	0001	000531	90L	0000	000103	904F	0003	011052	A
0004	000640	AM	0004	000705	AM1	0004	001135	ANUM	0004	000004	ATOM	0004	000514	BD
0004	000545	BOP	0005	000036	CALCH	0003	000000	COEF	0005	000000	CONVG	0006	000361	CPL
0004	000706	CPRI	0004	000634	CPSUM	0000	000000	CPUSED	0000	000000	CPX	0000	000007	CPXY
0004	000654	DATA	0003	010624	DECLN	0007	000002	DEMAND	0004	001560	DEMS	0003	000312	EN
0003	010150	ENLN	0004	001700	ENLSAV	0004	000000	ENM	0004	001676	ENHL	0004	001677	ENSAVE
0004	001414	ENTH	0004	000636	EQPAT	0004	001445	FAZ	0004	001527	FOX	0007	000000	GRAPH
0006	000551	HL	0005	000003	HP	0004	000642	HPP	0004	000637	HSUBD	0000	000034	HX
0000	000013	HXX	0003	010376	HO	0000	000037	I	0005	000010	IC	0005	000000	IDEBUG
0000	000001	IER	0000	000023	TEXTND	0006	001131	ILSP	0005	000015	IMAT	0000	000002	IMSG
0000	000132	INJPS	0005	000023	IONS	0005	000021	IP	0005	000037	ISAVE	0005	000016	ISL
0005	000005	ISV	0005	000034	IT	0003	016266	IUSE	0000	000026	IX	0005	000031	J
0005	000026	JL1Q	0007	000001	JOUT	0005	000025	J50L	0000	000024	K	0000	000025	KX
0005	000014	KMAT	0000	000027	KX	0004	000463	LLMT	0005	000040	LSAVE	0000	000036	M
0005	000006	MOLES	0004	000707	NAME	0005	000024	NC	0005	000022	NEWR	0005	000035	NFZ
0005	000012	NLM	0006	000000	NLISP	0005	000017	NOF	0005	000020	NOHIT	0005	000007	NP
0005	000011	NPT	0005	000027	NREAC	0005	000013	NS	0000	000000	NSPPI	0005	000010	NT
0000	000030	NTUP	0004	000635	OF	0004	001644	OYF	0004	001363	PECMT	0004	000633	PP
0004	000644	RH	0004	001611	RHOP	0004	001612	RMV	0004	001476	RTEMP	0003	000404	S
0005	000033	SHOCK	0006	000741	SL	0003	016660	SLN	0005	000004	SP	0003	015364	SUB
0006	000001	SUFLT	0004	000001	SUMN	0000	000033	SY	0000	000017	SXK	0004	000003	SD
0003	016514	TEMP	0004	000632	THIGH	0006	000171	TL	0004	000143	TLN	0000	000032	TLNS
0004	000630	TLOW	0004	000627	TM	0004	000631	TMID	0005	000002	TP	0004	000002	TI
0000	000031	TTS	0000	000003	TXX	0004	000646	VMIN	0005	000032	VOL	0004	000650	VPLS

000 000652 WP

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00101 1* SUBROUTINE CPHS 000002
00101 2* C CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES 000002
00101 3* C 000002
00101 4* C 000002
00101 5* C COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150) 000002
00101 6* C 1,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLN(150) 000002
00103 7* C INCLUDE SPECPC 000002
00107 8* C COMMON /MISC/ ENN,SUMM,TT,SD,ATOM(13,101),LLMT(25),BO(25), 000002
00107 9* C BO(25,2),TH,TLOW,TMID,THIGH,PP,CPSUM,OF,ECRAT, 000002
00107 10* C HSURD,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),MP(2), 000002
00107 11* C DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECWT(25), 000002
00107 12* C ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP, 000002
00107 13* C RHM(25),TLN,OXF(26),ENNL,ENSAVE,ENLSAV 000002
00110 14* C COMMON /INDX/ IDEBUG,CONVG,TP,HP,SP,ISV,MOLES,WP,NT,MPT,NLM,NS, 000002
00110 15* C KMAT,THAT,IO,NOF,NOMIT,IP,NEWR,IONS,NC,JSOL,JLTO, 000002
00110 16* C NREAC,IC,JVOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE 000002
00111 17* C COMMON /LOWTH/ NLTSP,SUBLT(40,3),TL(40,3),CPL(40,3),HL(40,3), 000002
00111 18* C SL(40,3),ILSP(40) 000002
00111 19* C 000002
00112 20* C COMMON /CCC/ GRAPH,JOUT,DEMAND 000002
00112 21* C 000002
00113 22* C DATA IER/O/,IMSG/-1/ 000002
00116 23* C DIMENSION IXX(4),CPXX(4),HXX(4),SXX(4) 000002
00117 24* C INTEGER SUB,SubLT 000002
00117 25* C 000002
00120 26* IEXTND = 0 000002
00121 27* IF (ITT,LT,TLOW) IEXTND = 1 000003
00123 28* IF (IEXTND.NE.O) IMSG = IMSG + 1 000011
00125 29* IF (IMSG.NE.O) GO TO 10 000016
00127 30* IF (IEXTND.NE.O) WRITE(JOUT,333) TT 000020
00133 31* 3333 FORMAT (/25X,NBLOW TEMPERATURE THERMO EXTENSION IN CPHS AT TT =, 000031
00133 32* 1 F12.6,15H DEGREES KELVIN//) 000031
00133 33* 10 K = 1 000032
00135 34* IF (ITT,LT,TMID) K=2 000040
00137 35* KK=0 000041
00140 36* CPSUM=0. 000043
00141 37* 20 IF (IUSE(K,1),J),NF.O,1 GO TO 30 000047
00143 38* IF (IUSE(J),LT,O) GO TO 40 000053
00145 39* KK=K 000055
00146 40* K=1 000057
00147 41* IF (KK.EQ.1) K=2 000065
00151 42* 30 IF (IEXTND.NE.O) GO TO 60 000067
00153 43* 31 S(J) = (((COEF(K,5,J)/4,0)*TT + COEF(K,4,J)/3,0)*TT + COEF(K,3,J)) 000114
00153 44* 1 /2,0)*TT + COEF(K,2,J))*TT + COEF(K,1,J)*TLN + COEF(K,7,J) 000114
00154 45* HO(J) = (((COEF(K,5,J)/5,0)*TT + COEF(K,4,J)/4,0)*TT + COEF(K,3,J)/3,0)*TT 000140
00154 46* 1*COEF(K,2,J)/2,0)*TT + COEF(K,1,J)*COEF(K,6,J)/TT 000157
00155 47* CPSUM = CPSUM + (((COEF(K,5,J))*TT + COEF(K,4,J))*TT + COEF(K,3,J))*TT + COEF(K, 000160
00155 48* IPIK,2,J))*TT + COEF(K,1,J))*EN(J,NPT) 000162
00157 49* 32 IF (KK.EQ.O) GO TO 40 000162
00160 50* K=KK 000162
00161 51* KK=0 000162

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CPHS

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00162 52* 40 IF (J, EQ, NS) RETURN
00163 53* J=J+1
00164 54* GO TO 20
00165 55* 60 IF (NLTSP, EQ, 0) GO TO 31
00166 56* 00 70 IX = 1, NLTSP
00167 57* 00 65 KX = 1, 3
00168 58* 65 IF (SUBJ, KX) .NE. SUBJ, (IX, KX) GO TO 70
00169 59* GO TO 80
00200 60* 70 CONTINUE
00201 61*
00202 62* 80 NTUP = 1, SP(IX)
00203 63* IE, IT, LI, YL(IX, 1) GO TO 90
00204 64* TFS = TT
00205 65* TLNS = TLN
00206 66* TT = TLOW
00207 67* TLN = ALOG(TT)
00208 68* KX = 2
00209 69* SX = ((1/COEF(KX, 5, J)/4) * TT + COEF(KX, 4, J)/3) * TT + COEF(KX, 3, J)/2)
00210 70* 1 * TT + COEF(KX, 2, J) * TT + COEF(KX, 1, J) * TLN * COEF(KX, 7, J)
00211 71* HX = ((1/COEF(KX, 5, J) * 5) * TT + COEF(KX, 4, J)/4) * TT + COEF(KX, 3, J)/3)
00212 72* 1 * TT + COEF(KX, 2, J)/2) * TT + COEF(KX, 1, J) * COEF(KX, 6, J) * TT
00213 73* CPX = ((1/COEF(KX, 5, J) * 5) * TT + COEF(KX, 4, J)/4) * TT + COEF(KX, 3, J)/3) * TT
00214 74* 1 * COEF(KX, 2, J) * TT + COEF(KX, 1, J)
00215 75* 00 86 KX = 1, NTUP
00216 76* TX(X, KX) = TL(IX, KX)
00217 77* CPX(X, KX) = CPL(IX, KX)
00218 78* HXX(KX) = HL(IX, KX)
00219 79* 86 SXX(KX) = SL(IX, KX)
00220 80* TX(X, NTUP, 1) = TT
00221 81* CPX(X, NTUP, 1) = CPX
00222 82* HXX(X, NTUP, 1) = HX
00223 83* SXX(X, NTUP, 1) = SX
00224 84* TT = TFS
00225 85* TLN = TLNS
00226 86* M = 1
00227 87* I = 1
00228 88* IF (IT, LT, TXX(M)) I = -1
00229 89* IF (IT, GE, TXX(M) .AND. TT .LE. TXX(M+1)) GO TO 89
00230 90* M = M + 1
00231 91* IF (M, LT, NTUP + 1 .AND. M, GT, 0) GO TO 87
00232 92* WRITE (JOUT, 88) TT, M, NTUP, (I, TXX(I), I = 1, 9)
00233 93* FORMAT (1/50X, 29H, CPHS, VARIABLE, OUTSIDE, TABLE//45X, 4HTT =, 1PE15.8
00234 94* 1, 5H, M =, 12, 8H, NTUP =, 12/150X, 4HTXX(1, 1, 3H) =, E15.8)
00235 95* GO TO 31
00236 96* STJ = SXX(M) + (SXX(M+1) - SXX(M)) * (TT - TXX(M)) / (TXX(M+1) - TXX(M))
00237 97* HQ(J) = HXX(M) + (HXX(M+1) - HXX(M)) * (TT - TXX(M)) / (TXX(M+1) - TXX(M))
00238 98* CPUSED = CPX(M) + (CPX(M+1) - CPX(M)) * (TT - TXX(M)) / (TXX(M+1) - TXX(M))
00239 99* CPSUM = CPSUM + CPUSED * ENJ, NPT)
00240 100* 60 TO 32
00241 101* IF (IER, LT, 1) WRITE (JOUT, 904) TT
00242 102* 904 FORMAT (1/25X, 40H, ERROR DURING LOW TEMPERATURE THERMO EVALUATION IN
00243 103* 1 CPHS, TT =, F12.6, 15H, DEGREES, CELSIUS//)
00244 104* IER = 1
00245 105* GO TO 31
00246 106* END

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CPHS

END OF COMPILATION:

NO DIAGNOSTICS.

3HUG.P

DETON

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BFOP'S DETON+DETONT
HSA E3 -10/15/80-13:06:18 (12.)

SUBROUTINE DETONT ENTRY POINT 001331

STORAGE USED: CODE(1) 001387; DATA(9) 000201; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 COMSTS 000006
0004 HOLCON 000010
0005 POINTS 000335
0006 MISC 001701
0007 INDX 000041
0010 PERF 000166
0011 OUP1 000013
0012 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0013 NEWOF
0014 HCLC
0015 OUF1
0016 EQLBRM
0017 OUT2
0020 OUT3
0021 SAVE
0022 NWOUS
0023 NI025
0024 XPRR
0025 EXP
0026 SORT
0027 NI015
0030 NI035
0031 NERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001305	1000L	0000	000035	11F	0001	000005	130G	0001	007040	146G	0001	000566	150L
0001	000053	154G	0000	000044	190F	0000	000053	203F	0001	000255	205L	0001	000176	214G
0000	000055	30F	0001	000651	141G	0001	000672	352G	0001	000711	362G	0001	000717	367G
0003	000367	40L	0001	000750	401G	0001	000767	411G	0001	001004	422G	0001	001024	433G
0003	001055	451G	0000	000114	46F	0001	001100	464G	0001	001115	475G	0000	000102	5F
0001	001123	507G	0001	001142	514G	0001	001157	525G	0001	001176	535G	0001	001216	546G
0000	000120	54F	0000	000123	68F	0001	000016	71L	0001	000615	860L	0000	000130	868F
0001	001251	874L	0001	001270	902L	0000	000032	ALAM	0000	000017	ALFA	0006	000640	AM
0006	000705	AM1	0006	001135	ANUM	0010	000133	APP	0003	000000	ATM	0006	000004	ATOM
0000	000022	AL1	0000	000023	412	0000	000024	A21	0000	000025	A22	0006	000514	BO
0006	000345	80F	0006	000026	81	0000	000027	B2	0007	000036	CALCH	0007	000001	CONVG
0005	000658	CF	0005	000032	CPR	0006	000706	CPR1	0006	000634	CP5UM	0012	000002	DEMAND
0006	001560	DEME	0005	000064	DLVPT	0005	000047	DLVTP	0004	000000	END	0006	001700	ENLSAV
0006	000000	ENN	0006	001676	ENML	0006	001677	ENSAVE	0006	0014	ENTH	0010	000165	EOL

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0005 000436 EQBAT 0011 000002 FA 0011 000003 FAP 0006 001445 FAZ 0011 R 000005 FB
0011 000007 FCP 0011 000012 FCST 0011 000014 FCV 0011 000015 FG
0011 000020 FGV 0000 R 000000 FGI 0011 R 000021 FHT 0011 000023 FI
0011 000025 FIV 0011 R 000027 FM 0000 R 000001 FHM 0011 R 000031 FMT 0011 000050 FN
0011 R 000052 FUR 0006 001527 FOX 0011 000053 FP 0000 R 000003 FPP 0000 R 000002 FPI
0000 R 000004 FRA 0000 R 000005 FRB 0011 000054 FS 0011 R 000056 FSV 0011 R 000057 FT
0011 000061 FTK 0000 R 000006 FTT 0011 000063 FV 0011 R 000065 FVEL
0011 R 000001 FL3 0011 000000 F9X 0000 R 000014 GAM 0005 R 000101 GAMMAS 0004 000001 GAS
0003 000001 GMEI 0010 R 000150 GM1 0012 000000 GRAPH 0007 L 000003 HP 0006 000642 HPP
0006 R 000637 HSUMO 0005 R 000000 HSUM 0010 R 000004 H1 0010 R 000004 H2 0007 I 000000 IDERUG
0004 000002 IE 0000 I 000011 II 0007 000015 IMAT 0007 000143 INJPS 0000 I 000010 IOF
0007 000023 IONS 0007 I 000021 IP 0007 000037 IOSAVE 0007 000016 IQ1 0007 I 000034 IT
0000 I 000012 ITR 0004 I 000003 IZERO 0000 I 000034 J 0007 000026 JLIQ 0012 I 000001 JOUT
0007 000025 JSUL 0007 000031 JS1 0007 I 000005 K 0007 000014 KMAT 0004 000004 LANK
0006 000463 LLMT 0007 000040 LSARE 0004 000005 MOL 0007 000006 MOLES 0006 I 000707 NAME
0007 000024 NC 0007 000022 NEUR 0007 000035 NF2 0007 000012 NLH 0007 I 000017 NOF
0007 000020 NOMIT 0007 I 000007 NP 0007 000011 NPT 0007 000027 NREAC 0007 000013 NS
0007 I 000010 NT 0006 R 000635 OF 0011 R 000067 ONE 0004 000006 OX 0006 R 001644 OXF
0005 R 000016 P 0003 000002 PATH 0010 R 000000 PCP 0006 001363 PCMT 0006 R 000633 PP
0005 R 000217 PPP 0000 R 000011 PPI 0010 R 000101 PUB 0003 R 000003 RRAR 0003 R 000004 RRR
0006 000644 RH 0004 001611 RHOP 0000 R 000020 RK 0006 001612 RMW 0010 R 000047 RRHO
0000 R 000021 RR1 0000 R 001476 RTEMP 0003 000005 RVR 0007 000033 SHOCK 0005 R 000251 SONVEL
0007 000004 SP 0005 000015 SSUM 0006 000001 SUMM 0006 000003 SO 0005 R 000150 T
0000 R 000016 TEM 0006 000632 THIGH 0011 R 000070 THREE 0006 001643 TLM 0006 000630 TLOW
0006 000637 TM 0006 000631 TM1D 0005 000320 TOTM 0007 L 000002 TP 0006 R 000002 TT
0005 R 000266 TTT 0000 R 000015 TTTD 0010 R 000116 TUB 0011 R 000071 TWO 0000 R 000033 UD
0005 R 000202 V 0005 000303 VLM 0006 000646 VM1N 0010 R 000032 VMOC 0007 000032 VOL
0006 000550 VPLS 0005 R 000234 VM 0006 000652 WP 0000 R 000030 X1 0000 R 000031 X2
0004 000007 ZERO 0011 000072 ZERO

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00101 10 SUBROUTINE DETON
00101 20 C
00101 30 C
00101 40 C
00103 50 COMMON /CONSTS/ ATMN,GMEI,PATM,RRAR,RRR,RVR
00104 60 COMMON /HOLCON/ END,GAS,IE,IZERO,LANK,MOL,OX,ZERO
00105 70 COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
00105 80 1 ,GAMMAS(13),PI(26),T(26),V(13),PP(13),WM(13),SONVEL(13),TTTT(13)
00105 90 2 ,VLM(13),TOTM(13)
00106 100 COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(13,101),LLMT(25),BO(25),
00106 110 BO(25,2),TM,TLOW,THID,THIGH,PP,CP,SUM,OF,EORAT,
00106 120 HSURD,AM(2),HPP(2),RH(2),VMIN(2),VPLS(2),VP(2),
00106 130 CP(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECMT(25),
00106 140 ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENS(25),RHOP,
00106 150 RMW(25),ILN,OXE(26),ENNL,ENSARE,ENLSAV
00107 160 COMMON /INDX/ IDERUG,CONVS,TP,HP,SP,K,MOL,MP,NT,NPT,NLM,NS,
00107 170 KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEUR,IONS,NC,JUL,JLIO,
00107 180 NREAC,IC,J31,VOL,SHOCK,I,NF2,CALCH,IOSAVE,LSAVE
00107 190 COMMON /PERF/ PCPI(26),VMOC(13),RRHO(13),H(13),PUB(13),
00107 200 TUB(13),APPL(13),GM(13),EQL
00107 210 COMMON /OUP/ F9X,F13,FA,FAP(2),FB,FC,FCPI(3),FCST(2),FCV,FG(2),
00107 220 FGE,FGV,FH(2),FII(2),FIV(2),FMI(2),FMT(15),FM(2),FOUR,
00107 230 FP,FS(2),FSV,FT(2),FTR(2),FV(2),FVEL(2),FONE,THREE,

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DETON

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00111 24* 3 TW0,ZEP0F /OUP1/ 000000
00111 25* C COMMON /CCC/ GRAPH,JOUT,DEMAND 000000
00112 26* C LOGICAL EOL,MP,TP 000000
00113 27* C DATA FG,SGAMMA1,FMH,GMH,M1,J,P1,6HP1,ATN,FPP,6HP,P1, 000000
00114 28* C 1 FRA/6HND/RH,FRB/6H01 /,FIT/6HT/T1 /,FUD/6HDET VE/ 000000
00115 30* C XX(A,Y,B,V,C,D) = (A*X-B*Y)/(A*C-B*D) 000000
00116 31* C IOF = 0 000000
00117 32* C DO 11 I=1,NREAC 000000
00118 33* C * NAME(I,6)=ZERO 000005
00119 34* C TT = 0. 000007
00120 35* C IF (TT) .LE. 0.0) TT(1) = RTEMP(1) 000010
00121 36* C 7 IOF = IOF+1 000016
00122 37* C OF = OF(I OF) 000021
00123 38* C CALL NEWOF 000023
00124 39* C WRITE(JOUT,11) 000025
00125 40* C 11 FORMAT(3H10 DETONATION VELOCITY CALCULATIONS) 000032
00126 41* C CO 902 IT = 1,M 000032
00127 42* C TT = TT(1) 000040
00128 43* C CALL HCALL 000042
00129 44* C CALL OUT1 000044
00130 45* C DO 902 IP=1,MP 000046
00131 46* C H1(NPT) = RBAR*HSUBO 000055
00132 47* C TUB(NPT) = T(IT) 000061
00133 48* C PUB(NPT) = P(IT) 000063
00134 49* C CP(NPT) = RBAR*CPRI 000065
00135 50* C ITR = 0 000070
00136 51* C TT = 3800. 000071
00137 52* C PP = PP1*P(IT) 000073
00138 53* C HSUBO = H1(NPT)/RBAR + 0.750*TT(1)*PP1/AMI 000075
00139 54* C TP = .FALSE. 000077
00140 55* C HP = .TRUE. 000105
00141 56* C CALL EOLBPH 000106
00142 57* C HSUBO = H1(NPT)/RBAR 000110
00143 58* C HP = .FALSE. 000117
00144 59* C IF (TT .LE. 0.0) GO TO 902 000123
00145 60* C GAM = GAMMA5(NPT) 000126
00146 61* C TT = TT/TT(1) 000137
00147 62* C IT = 0 000142
00148 63* C TEM=TT-.75*PP1/(CPR(NPT)*AMI) 000143
00149 64* C WRITE(JOUT,190)TT 000150
00150 65* C 190 FORMAT(8H01 EST.-,F8.2/11X,4HP/P1,17X,4HT/T1) 000160
00151 66* C WRITE(JOUT,203) IT,PP1,TT 000160
00152 67* C DO 202 II = 1,3 000176
00153 68* C ALFA = WM(NPT)/AM2/TT1 000176
00154 69* C PP1 = (1.+GAM)*0.1+.11.-N.*GAM*ALFA/(1.+GAM)*0.2**5)/(12.*GAM*ALFA) 000201
00155 70* C RK=PP1*ALFA 000220
00156 71* C TT1 = TEM+.5*PP1*GAM*(RK*RK-1.)/(AMI*CP(NPT)*RK) 000222
00157 72* C 202 WRITE(JOUT,203) IT,PP1,TT1 000223
00158 73* C 203 FORMAT(15,2E20.8) 000235
00159 74* C TP = .TRUE. 000247
00160 75* C TT = TT1+1.1) 000251

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00233 800 205 ITR= ITR+1
00234 810 PP = PPI*P(IP)
00235 820 CALL EQLBRM
00236 830 IF (NPT.EQ.0) GO TO 1000
00240 840 IF (IT .LE. 0.0) GO TO 860
00242 850 GAM = GAM*ASIN(NPT)
00243 860 PPI = PPI*VM(NPT)/AML/ITI
00244 870 A11 = 1./PPI + GAM*RR1*OLVTP(NPT)
00245 880 A12 = GAM*RR1*OLVTP(NPT)
00246 890 A21 = 5.*GAM*(RR1**2-1.-OLVTP(NPT)*(1.-RR1**2))*OLVTP(NPT)-1.
00247 900 A22 = -5.*GAM*OLVTP(NPT)*(RR1**2-1.-VM(NPT))*CPR(NPT)
00250 910 B1 = 1./PPI-1.-GAM*(RR1-1.)
00251 920 B2 = VM(NPT)*INSUM(NPT) - W1(NPT)/RRAR1/ITI - 0.5.*GAM*(RR1**2 - 1.)
00252 930 X1 = XX(A22-B1*A12-B2*A11,A21)
00253 940 X2 = XX(A11,B2,A11,B1,A22,A12)
00254 950 ALAM = 1.
00255 960 TEM = X1
00256 970 IF (TEM.LT.0.) TEM = -TEM
00257 980 IF (X2.GT.TEM) TEM=X2
00262 990 IF (-X2.GT.TEM) TEM = -X2
00264 1000 IF (TEM.GT.0.) ALAM = 4/TEM
00266 1010 PPI = PPI*EXP(X1*ALAM)
00267 1020 Y1 = Y1*EXP(X2*ALAM)
00270 1030 Y1 = Y1*Y1
00271 1040 UD = RR1*SORT(RR*GAM*ATT/VM(NPT))
00272 1050 WRITE(JOUT,30) ITR,PPI,ITI,RR1,X1,X2
00302 1060 30 FORMAT(IHOUTER = I2,5X,6HP/PI = E15.8,5X,6HT/ITI = E15.8,5X,10MRHO/
00302 1070 1RH01 = E15.8,7X,13HDEL LN P/PI = E15.8,5X,13HDEL LN I/ITI = E15.8)
00302 1080 C CONVERGENCE TEST
00303 1090 IF (ITR.LT.10 .AND. TEM.GT.0.5E-04) GO TO 205
00305 1100 RPH0(NPT)=RR1
00306 1110 IF (CP(NPT) .LE. 0.0) GO TO 40
00310 1120 GM1(NPT) = CP(NPT)/(CP(NPT) - RRAR/AM1)
00311 1130 VMC(NPT) = UD/SORT(RR*GAM1(NPT)*Y1/ITI)/AM1)
00312 1140 GO TO 150
00313 1150 40 GM1(NPT) = 0.
00314 1160 VMC(NPT) = 0.
00315 1170 150 K = 0
00316 1180 IF (IP .EQ. NP .AND. IT .EQ. NT .OR. IT .LE. 0.0) GO TO 860
00320 1190 K = NPT
00321 1200 IF (NPT.NE.13) GO TO 870
00321 1210 C OUTPUT
00323 1220 860 WRITE(JOUT,5)
00325 1230 5 FORMAT(IH1,R2X,46HDETONATION PROPERTIES OF AN IDEAL PEACTING GAS )
00326 1240 CALL OUT1
00331 1250 46 WRITE(JOUT,46)
00332 1260 FMT(1) = F13
00333 1270 FMT(4) = F04
00334 1280 WRITE(JOUT,FMT) PPI,FB,FB,(PUBI,J), J = 1,NPT)
00345 1300 FMT(4) = F04
00346 1310 WRITE(JOUT,FMT) F1,FB,(TUB(J), J = 1,NPT)
00356 1320 WRITE(JOUT,FMT) F4,FB,(H1(J), J = 1,NPT)
00366 1330 DO 56 J = 1,NPT
00371 1340 V1(J) = AM1
00372 1350 56 SONVEL(I,J) = SORT(RR*GAM1(J)*TUB(J)/AM1)

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DETON

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00374 136* FMT(4) = THREE 000732
00375 137* WRITE(JOUT,FMT) FM,FB,(V(J), J = 1,NPT) 000734
00405 138* FMT(4) = FOUR 000753
00406 139* WRITE(JOUT,FMT) FCP,ICP(J), J = 1,NPT) 000755
00415 140* WRITE(JOUT,FMT) FG,FB,FB,(GM(J), J = 1,NPT) 000772
00426 141* FMT(4) = ONE 001007
00427 142* WRITE(JOUT,FMT) FSV,FVEL,(SONVEL(J), J = 1,NPT) 001011
00437 143* WRITE(JOUT,58) 001027
00441 144* 58 FORMAT(11'HURNED GAS//) 001034
00442 145* FMT(3) = ONE 001034
00443 146* CALL OUT2 001036
00444 147* WRITE(JOUT,68) 001040
00446 148* 68 FORMAT(22'MODE,ONATION PARAMETERS //) 001050
00447 149* FMT(4) = THREE 001050
00450 150* DO 70 J = 1,NPT 001055
00453 151* V(J) = PPP(J)/PUB(J) 001055
00454 152* PCP(J) = TTT(J)/TUR(J) 001057
00455 153* 70 SONVEL(J) = SONVEL(J)ORRHOL(J) 001062
00457 154* WRITE(JOUT,FMT) FFP,FB,FB,(V(J), J = 1,NPT) 001066
00470 155* WRITE(JOUT,FMT) FIT,FB,FB,(PCP(J), J = 1,NPT) 001103
00501 156* DO 73 J = 1,NPT 001123
00509 157* V(J) = MM(J)/AM1 001126
00506 158* FMT(4) = FOUR 001130
00507 159* WRITE(JOUT,FMT) FMM,FB,FB,(V(J), J = 1,NPT) 001145
00520 160* WRITE(JOUT,FMT) FRA,FB,FB,(RRHOL(J), J = 1,NPT) 001162
00531 161* FMT(4) = ONE 001201
00542 162* WRITE(JOUT,FMT) FUD,FVEL,(SONVEL(J), J = 1,NPT) 001203
00552 163* EQL = .TRUE. 001221
00553 164* CALL OUT3 001223
00554 165* IF (K.EQ.0.AND. IOF.EQ.NCF) GO TO 1000 001225
00556 166* IDEBUG = IDEBUG-13 001237
00557 167* WRITE(JOUT,68) 001242
00561 168* 68 FORMAT(11H) 001247
00562 169* NPT = 0 001247
00563 170* 870 NPT = NPT + 1 001251
00564 171* IF (K.EQ.1) K = -1 001253
00566 172* CALL SAVE 001260
00567 173* WRITE(JOUT,68) 001262
00571 174* 902 CONTINUE 001274
00574 175* IF (IOF.EQ.NCF) GO TO 1000 001274
00576 176* IDEBUG = IDEBUG+13 001300
00577 177* GO TO 7 001303
00600 178* 1000 TP = .FALSE. 001305
00601 179* RETURN 001305
00602 181* END 001346

```

END OF COMPILATION: NO DIAGNOSTICS.

DEBUG.P EQU.BRM

EOLBRM

FOR'S EOLBRM,EOLBRM
MSA E3 -10/15/80-13:06:23 (16,)

SURROUTINE EOLBRM ENTRY POINT 003120

STORAGE USED: CODE(1) 003136: DATA(0) 000461: BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCON 000010
0005 POINTS 000335
0006 SPECES 017106
0007 MISC 001701
0010 DOUBLE 001960
0011 INDY 000041
0012 PERF 000166
0013 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0014 CP'S
0015 MATRIX
0016 GAUSS
0017 ALOG
0020 NVDUS
0021 NIOIS
0022 NIOZS
0023 EXP
0024 MERRIS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001202	100L	0001	001211	101L	0001	002172	10276	0001	002222	10376	0000	000213	110F
0001	001452	111L	0001	001575	1115L	0001	001633	1116L	0001	001517	113L	0001	002503	11346
0001	001513	114L	0001	002511	11406	0001	001542	115L	0001	002551	11546	0001	003660	116L
0001	002624	1160L	0001	002454	1165L	0001	002716	1171L	0000	000214	1183F	0001	002644	1205G
0001	002676	12236	0001	002741	12446	0001	002046	13L	0000	003747	130L	0000	000321	136F
0001	002660	143L	0000	000257	144F	0001	002263	147L	0001	002270	148L	0001	000116	151G
0001	002516	153L	0001	002312	154L	0000	000265	156F	0001	002342	157L	0001	002401	158L
0001	002437	159L	0001	002152	160L	0000	000277	161F	0001	000151	1656	0001	002630	165L
0001	002650	166L	0000	000307	168F	0001	002616	169L	0001	002521	170L	0001	002725	171L
0000	000111	172F	0001	000430	174L	0001	002002	183L	0001	003013	186L	0000	000165	1924F
0001	003002	199L	0000	000326	201F	0001	001561	2115L	0001	000244	2216	0001	000277	2326
0000	000072	244F	0001	000325	245G	0001	000332	251G	0001	000374	2706	0001	000406	2776
0000	000220	306F	0001	000464	315G	0001	000512	3246	0001	000131	33L	0001	000613	360G
0000	000103	373F	0001	002653	40L	0001	000721	416G	0001	000732	4226	0001	000155	43L
0001	001003	445G	0001	001141	477G	0001	000125	499L	0001	001172	506G	0001	001252	5316
0001	001413	600G	0001	000213	62L	0001	000251	63L	0001	001464	6316	0001	000302	67L
0001	001625	673G	0001	001642	704G	0001	000342	72L	0001	001722	7266	0000	000107	73F
0000	000140	74F	0001	001760	746G	0000	000324	771F	0000	000075	772F	0001	000412	773L
0001	000524	774L	0001	000536	775L	0000	000144	776F	0001	000747	80L	0001	000766	83L

ORIGINAL PAGE IS
OF POOR QUALITY

EOLBAM

0001	001023 04L	0001	001036 05L	0001	000571 071L	0001	003071 073L	0000	000117 074F
0001	001332 917L	0000	000146 923F	0000	000171 924F	0000	000210 925F	0001	000403 966L
0001	000622 960L	0001	000632 969L	0001	001111 971L	0001	000635 970L	0001	000644 971L
0000	000232 973F	0000	000250 974F	0001	000659 977L	0006	001055 978L	0000	000061 AA
0001	000150 AEAT	0007	000640 AM	0000	000054 AMBDA	0000	000055 AMBDA1	0007	000705 AM1
0001	001135 ANUM	0012	000131 AP	0000	000000 ATMM	0007	000000 ATOM	0007	000014 BQ
0007	000345 BOP	0011	000036 CALCH	0000	000000 COEF	0011	000001 COMV6	0005	000032 CPR
0007	000706 CPRI	0007	000036 CPSUM	0000	000040 CRITV	0007	000054 DATA	0000	000047 DELF
0006	001624 DELM	0013	000002 DEMAND	0007	01560 DEMS	0000	000053 DLMT	0005	000044 DLYPT
0005	000047 DLYTP	0006	000312 EN	0004	000000 END	0007	000037 ENL	0006	001050 ENCL
0007	001700 ENLSAV	0007	000000 ENN	0007	001676 ENML	0007	001677 ENSAVE	0000	000045 ENSOL
0007	001919 ENIM	0012	000165 EBL	0007	000636 EORAT	0007	001445 FAZ	0000	000087 FNEG1
0000	000060 FNEG2	0007	001927 FOX	0010	000000 G	0005	000011 GAMMAS	0004	000001 GAS
0003	000001 GMEY	0013	000000 GRAPH	0011	000003 HP	0007	000642 HPP	0007	000637 HSUBD
0005	000000 HSUM	0006	0010376 HO	0000	000044 I	0011	000030 IC	0011	000000 IDEBUG
0004	000002 IE	0011	000015 IMAT	0000	000063 IMC	0000	000421 IMJPS	0011	000023 IOMS
0011	000021 IP	0011	000037 IOSAVE	0011	000016 IQ1	0000	000047 IO2	0000	000034 ISIMG
0011	000021 ISV	0011	000024 IT	0000	000042 ITMUMB	0006	001626 IUSE	0004	000003 IZERO
0000	000043 J	0000	000070 JOELF	0000	000051 JJ	0000	000065 JNG	0011	000026 JLIO
0011	000001 JOYT	0011	000025 JSOL	0011	000031 JS1	0000	000044 KE	0011	000019 KMAY
0011	000012 L	0004	000004 LANK	0007	000043 LLMT	0000	000035 LO6V	0011	000040 LSAVE
0009	000005 MOL	0011	000006 MOLES	0007	000707 NAME	0011	000024 NC	0000	000052 MEM
0011	000022 MEWR	0011	000035 MIZ	0011	000017 MOF	0011	000020 MOMIT	0011	000007 MP
0011	000011 MPI	0011	000027 MNEAC	0011	000013 MS	0000	000000 MSPJ3	0011	000010 MT
0000	000050 MYZERO	0000	000046 MUMB	0007	000635 OF	0004	000006 OX	0007	001644 OXF
0005	000016 P	0003	000002 PATH	0012	000000 PCP	0007	001363 PECVT	0007	000633 PP
0005	000217 PPP	0000	000001 PROV	0003	000000 RBAR	0003	000004 RBR	0007	000644 RH
0007	001611 RHOP	0000	000036 RTE	0007	001612 RMV	0007	001476 RTEMP	0003	000005 RVR
0006	000064 S	0011	000033 SMOCK	0000	000041 SIZEF	0006	016660 SLW	0003	000251 SONVEL
0011	000004 SP	0012	000047 SPIM	0000	000042 SS	0005	000015 SSUM	0006	0015364 SUB
0012	0000101 SUBAR	0000	000032 SUM	0007	000001 SUMN	0000	000056 SUM1	0012	000116 SUPAR
0007	000003 SO	0003	000150 Y	0006	001614 TEMP	0007	000632 THIGH	0007	0001643 TLM
0007	000030 TLOW	0007	000627 TM	0000	000066 TMELT	0007	000631 TMID	0000	000071 TM
0005	000320 TOTM	0011	000002 TP	0007	000002 TT	0005	000266 TTT	0005	000202 V
0012	000064 VACI	0005	000103 VLM	0007	000646 VHM	0012	000032 VMOC	0011	000032 VOL
0007	000050 VPLS	0005	000234 VM	0007	000652 VP	0010	0001510 X	0004	000007 ZERO

00101	10	SUBROUTINE EOLBAM		EOLM0002	0000000
00101	20	C	ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES	EOLM0003	0000000
00101	30	C		EOLM0004	0000000
00101	40	C	COMMON /CONSTS/ ATMM,CHET,PATH,RBAR,RBR,RVR	/CONSTS/	0000000
00103	50		COMMON /MOLCON/ ENO,GAS,IE,IZERO,LANK,MOL,OX,ZERO	/MOLCON/	0000000
00104	60		COMMON/POINTS/HSUM(13),SSUM(13),CPRI(13),DLYTP(13)		0000000
00105	70		1 ,GAMMAS(13),P(26),T(26),Y(13),PP(13),MM(13),SONVEL(13),JTL(13)		0000000
00105	80		2 ,VLM(13),TOTM(13)		0000000
00105	90		COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLMI(150),MD(150)		0000000
00105	100	C	1 ,DELMI(150),A(15,150),SUB(150,3),IUSE(150,2),SLMI(150)		0000000
00105	110	C	INCLUDE SPECPR		0000000
00106	120		COMMON /MISC/ ENN,SUMN,TT,SO,ATOM(3,101),LLMT(25),BOR(25),		0000000
00112	130		00P(25,2),JM,TLOW,TMID,THIGH,PP,CPSUM,OF,EORAT,		0000000
00112	140		HSUBD,AM(2),MPP(2),RH(2),VMIN(2),VPLS(2),MPI(2),	/MISC/	0000000
00112	150		DATA(25),AM1,CPRI,NAME(25,6),ANUM(25,6),PECUT(25),		0000000
00112	160				0000000

EOLBEM

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00112 170      EMT(25),FAZ(25),RTMP(25),FOX(25),DEMS(25),RMOP,
00112 180      RMU(25),ILN,OFF(26),ENML,ENSAVE,ENLSA
00113 190      COMMON /DOUBLE/ G(20,2), X(20)
00114 200      COMMON /INDX/ IDEBUG,COM,G,TP,MP,SP,ISV,MOLES,MP,NT,NPT,L,MS,
00114 210      RMAT,IMAT,IOI,MO,MONIT,TP,NEW,IONS,NC,JSOL,JL10,
00114 220      HREAC,IC,JSI,VOL,SHOCK,TF,MFZ,CALCM,LOGAVE,LSAVE,
00115 230      COMMON /PERF/ PCP(26),VROC(13),SPIM(13),VACI(13),SUNAP(13),
00115 240      SUPAR(13),APP(13),AEAT(13),EOL
00115 250      C
00116 260      COMMON /CCC/ GRAPH,JOUT,DEMAND
00116 270      C
00117 280      DIMENSION PROM(25)
00120 290      DOUBLE PRECISION G,SUM,X
00121 300      LOGICAL CMVG,MP,IC,IONS,ISING,LOGV,RITE,SHOCK,SP,TP,VOL
00121 310      C
00122 320      EML = ENML
00123 330      RITE = .FALSE.
00123 340      IEIDEBUG,GT,0,AMD,NPT,GE,IDEBUG, RITE=.TRUE.
00126 350      CRITY = 5.0E-6
00127 360      SIZEF = 0.
00130 370      ISING = .FALSE.
00131 380      LOGV = .FALSE.
00132 390      IF (VOL) SP = RVROEMM*TP/VLM(MPT)
00134 400      TLM = ALOG(1)
00135 410      CMVG = .FALSE.
00136 420      ITNUMB = 100
00137 430      JSI = 1
00140 440      CALL CPMS
00141 450      TM = ALOG(P/ENM)
00141 460      IF(JCI) PREVIOUS_POINT HAD SINGULAR MATRIX
00142 470      IF(ICI) GO TO 966
00144 480      IF (I.NOT.IONS,OR,IE.EQ.LLMT,I) GO TO 33
00146 490      L = L+1
00147 500      IOI = IOI+1
00150 510      DO 499 J = 1,NS
00153 520      IF (FAIL,J).EQ.D,1 GO TO 999
00155 530      ENJ,MPT) = 1.E-8
00156 540      ENJ,MPT) = -10.-206610
00157 550      IUSE(J) = 0
00160 560      999 CONTINUE
00162 570      33 IF(MPT.EQ.1,AMD,.NOT.SHOCK) WRITE(JOUT,200) (LLMT(I),I=1,L)
00171 580      200 FORMAT (TEMP,14(SX,A))
00171 590      C BEGIN ITERATION
00172 600      43 IF(ICI) GO TO 1171
00174 610      IF I.NOT.CMVG) GO TO 62
00176 620      SUM = ENM
00177 630      IF(JSOL.EQ.0) GO TO 62
00201 640      ENSOL = ENJSOL,MPT)
00203 650      ENJSOL,MPT) = ENJSOL,MPT)+ENJLIO,MPT)
00203 660      IUSE(JLIO) = -IUSE(JLIO)
00204 670      IOI = IOI-1
00205 680      DLTP(MPT) = 0.
00206 690      CPRINTP) = 0.
00207 700      GAMMA(SIMP) = 0.
00210 710      LOGV = .TRUE.
00211 720      62 CALL MATRIX

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EOLM0004

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00212 730 NUMB = 101 - ITHUMB
00213 740 I02 = 101 + 1
00214 750 IF (.NOT. CONV) GO TO 67
00215 760 IF (LOGV.AND..JOL.EQ.0) GO TO 63
00216 770 DO 162 I=1,L
00217 780 PROM(I) = G(I01,I)
00218 790 IF (.NOT. LOGV) GO TO 67
00219 800 LOGV = .TRUE. -- SET UP MATRIX TO SOLVE FOR DLVPT
00220 810 63 G(I01,I02) = ENN
00221 820 J = I01 - 1
00222 830 DO 777 I = 1,J
00223 840 777 G(I,I02) = G(I,I01)
00224 850 67 IF (.NOT. RITE) GO TO 72
00225 860 WRITE(JOUT,777) NUMB
00226 870 772 FORMAT (11HQUATION ,13,6X,7HMATRIX //)
00227 880 DO 911 I=1,IMAT
00228 890 9.1 WRITE(JOUT,73) (G(I,J), J = 1,IMAT)
00229 900 72 IF (CONV) IMAT=IMAT-1
00230 910 J = IMAT
00231 920 CALL GAUSS
00232 930 IF (J .NE. IMAT) GO TO 774
00233 940 IF (.NOT. RITE) GO TO 773
00234 950 WRITE(JOUT,733) (LMT(I), I=1,L)
00235 960 773 FORMAT (11HOP ,91A,10X)
00236 970 WRITE(JOUT,733) (X(I), I=1,IMAT)
00237 980 73 FORMAT (9E10,6)
00238 990 773 IF (.NOT. CONV) GO TO 85
00239 1000 IF (.NOT. LOGV) GO TO 174
00240 1010 IF (JLO.NE.O) ENJSOL(MPT)=ENSO
00241 1020 GO TO 171
00242 1030 174 SUM = 0.
00243 1040 DO 175 J=1,L
00244 1050 175 SUM = SUM + PROV(J)*X(J)
00245 1060 DLVTP(MPT) = 1.-G(I02,I01)/ENH-SUM/ENN - X(I01)
00246 1070 CPR(MPT) = G(I02,I02)
00247 1080 DO 176 J=1,I01
00248 1090 176 CPR(MPT) = CPR(MPT) - G(I02,J)*X(J)
00249 1100 LOGV = .TRUE.
00250 1110 GO TO 62
00251 1120 C SINGULAR MATRIX
00252 1130 774 IF (.NOT. CONV) GO TO 775
00253 1140 C IF (ISING) SINGULAR ONCE
00254 1150 C IF (IC) SINGULAR TWICE
00255 1160 WRITE(JOUT,172)
00256 1170 172 FORMAT(2HDERIVATIVE MATRIX SINGULAR )
00257 1180 IC = .TRUE.
00258 1190 GO TO 1171
00259 1200 775 IF (.NOT. MP.OP.MPT.NE.1.OR.NC.EQ.0.OR.JT.GT.100.) GO TO 871
00260 1210 WRITE(JOUT,874)
00261 1220 874 FORMAT(6HLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
00262 1230 BEEN INCLUDED ON AN INSERT CARD. RESTART )
00263 1240 GO TO 873
00264 1250 871 WRITE(JOUT,74)
00265 1260 74 FORMAT(16H0 SINGULAR MATRIX)
00266 1270 IF (IC) GO TO 873
00267 1280 IF (ISING) GO TO 997
00268 1290
00269 1300
00270 1310
00271 1320
00272 1330
00273 1340
00274 1350
00275 1360
00276 1370
00277 1380
00278 1390
00279 1400
00280 1410
00281 1420
00282 1430
00283 1440
00284 1450
00285 1460
00286 1470
00287 1480
00288 1490
00289 1500
00290 1510
00291 1520
00292 1530
00293 1540
00294 1550
00295 1560
00296 1570
00297 1580
00298 1590
00299 1600
00300 1610
00301 1620
00302 1630
00303 1640
00304 1650
00305 1660
00306 1670
00307 1680
00308 1690
00309 1700
00310 1710
00311 1720
00312 1730
00313 1740
00314 1750
00315 1760
00316 1770
00317 1780
00318 1790
00319 1800
00320 1810
00321 1820
00322 1830
00323 1840
00324 1850
00325 1860
00326 1870
00327 1880
00328 1890
00329 1900
00330 1910
00331 1920
00332 1930
00333 1940
00334 1950
00335 1960
00336 1970
00337 1980
00338 1990
00339 2000
00340 2010
00341 2020
00342 2030
00343 2040
00344 2050
00345 2060
00346 2070
00347 2080
00348 2090
00349 2100
00350 2110
00351 2120
00352 2130
00353 2140
00354 2150

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EQ, BPM

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00356 1290
00357 1300
00358 1310
00359 1320
00360 1330
00361 1340
00362 1350
00363 1360
00364 1370
00365 1380
00366 1390
00367 1400
00368 1410
00369 1420
00370 1430
00371 1440
00372 1450
00373 1460
00374 1470
00375 1480
00376 1490
00377 1500
00378 1510
00379 1520
00380 1530
00381 1540
00382 1550
00383 1560
00384 1570
00385 1580
00386 1590
00387 1600
00388 1610
00389 1620
00390 1630
00391 1640
00392 1650
00393 1660
00394 1670
00395 1680
00396 1690
00397 1700
00398 1710
00399 1720
00400 1730
00401 1740
00402 1750
00403 1760
00404 1770
00405 1780
00406 1790
00407 1800
00408 1810
00409 1820
00410 1830
00411 1840
00412 1850
00413 1860
00414 1870
00415 1880
00416 1890
00417 1900
00418 1910
00419 1920
00420 1930
00421 1940
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00505 1850 DO 99 J = 1,L
00510 1850 DELM(J) = DELM(J) * A(I,J)*X(I)
00515 1850 GO TO 101
00520 1850 DELM(J) = X(I,J)
00525 1850 JJ = JJ + 1
00530 1850 CONTINUE
00535 1850 AMBDA = 1.
00540 1850 SUM = X(I,0)
00545 1850 IF (SUM - 1.0) SUM = -SUM
00550 1850 IF (DELMT.GT.SUM) SUM = DELMT
00555 1850 IF (DELMT.GT.SUM) SUM = -DELMT
00560 1850 DO 917 J = 1,MS
00565 1850 IF (IUSE(J).NE.0) GO TO 917
00570 1850 IF (IEM(J,MPT) .GT. 0.0 .AND. DELM(J) .GT. SUM) SUM = DELM(J)
00575 1850 IF (IEM(J,MPT) .GT. 0.0 .OR. DELM(J) .LE. 0.0) GO TO 917
00580 1850 SUM = (-9.212 * EML(J) * EML) / (DELM(J) - X(I,0))
00585 1850 IF (SUM - 1.0) SUM = -SUM
00590 1850 IF (SUM - 1.0) AMBDA = SUM
00595 1850 917 CONTINUE
00600 1850 IF (SUM - 2.0) AMBDA = 2.0 / SUM
00605 1850 IF (AMBDA - 1.0) AMBDA = AMBDA
00610 1850 IF (NOT (RITE)) GO TO 111
00615 1850 WRITE (JOUT, 923) I, EML, EML, PP, I, AMBDA
00620 1850 923 FORMAT (1X, I = 1, EML = E15.8, M = E15.8, 7H EML = E15.8, 5H PP = E15.8,
00625 1850 1 9H LN P/M = E15.8, 8H AMBDA = E15.8)
00630 1850 IF (VOL) WRITE (JOUT, 192) VLM, MPT
00635 1850 192 FORMAT (1X, VOLUME = E15.8, 2HCC)
00640 1850 924 FORMAT (1X, I = 1, 2H I, 12H SM, M = 1, 8H NI, 10H, 9H H/MT, 9H, 9H SO /
00645 1850 1 12H, 6H - GO / RT, 9H, 5H - G / RT)
00650 1850 DO 926 J = 1, MS
00655 1850 FMEG1 = S(I) - M(J)
00660 1850 FMEG2 = FMEG1
00665 1850 IF (IUSE(J).EQ.0) FMEG2 = FMEG2 - EML(J) - Y
00670 1850 926 WRITE (JOUT, 925) SUM(J, 1), SUB(J, 2), SUB(J, 3), EML(J, MPT), EML(J, 1),
00675 1850 A DELM(J), M(J), S(I), FMEG1, FMEG2
00680 1850 925 FORMAT (1X, 3A, 7E15.6)
00685 1850 WRITE (JOUT, 110)
00690 1850 110 FORMAT (1X, 0)
00695 1850 C APPLY CORRECTIONS TO ESTIMATES
00700 1850 111 SUM = 0.
00705 1850 DO 113 J = 1, MS
00710 1850 IF (IUSE(J)) 113, 112, 114
00715 1850 112 EML(J) = EML(J) - AMBDA * DELM(J)
00720 1850 EML(J, MPT) = 0.
00725 1850 IF (EML(J) * 10.4206810 .LE. EML) GO TO 113
00730 1850 EML(J, MPT) = EXP(EML(J))
00735 1850 SUM = SUM + EML(J, MPT)
00740 1850 GO TO 113
00745 1850 114 EML(J, MPT) = EML(J, MPT) AMBDA * DELM(J)
00750 1850 113 CONTINUE
00755 1850 SUM = SUM
00760 1850 IF (IPI) GO TO 115
00765 1850 TLM = TLM - AMBDA * DELMT
00770 1850 IT = EXP(IPI)
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01010 2970 WRITE (JOUT,970) TT
01013 2980 970 FORMAT (5X,'3000 TEMPERATURE=','F12.0',' 3000')
01016 2990 IF (I-NOT-4-OR-MPT-ME-1-OR-MC-EO-0-OR-TT-67.100.) GO TO 873
01020 3000 WRITE (JOUT,870)
01021 3010 TT = T111
01022 3020 RETURN
01023 3030 C CONVERGENCE TESTS ARE SATISFIED. TEST CONDENSED SPECIES.
01024 3040 160 IF (MC-EO-0) GO TO 103
01025 3050 SIZEF = 0.
01026 3060 IMC = 0
01027 3070 DO 170 J = 1,MS
01028 3080 IF (IUSE(J),EQ-0 .OR. IUSE(J),EQ-100001 GO TO 170
01029 3090 IMC = IMC +
01030 3100 IF (IMC) WRITE (JOUT,100) (SUB(J,1),1=1,3),TEMP(INC,2),
01031 3110 IUSE(J),EN(J,MPT)
01032 3120 100 FORMAT (10D,3A,2F10.3,3X,SMIUSE=,10,E15.7)
01033 3130 IF (EN(J,MPT)) 106,108,109
01034 3140 106 IF (J-MC-JSOL-AND-J-ME-JLIQ) GO TO 107
01035 3150 JSOL = 0
01036 3160 JLIQ = 0
01037 3170 107 101 = 101 - 1
01038 3180 EN(J,MPT) = 0.
01039 3190 GO TO 108
01040 3200 108 NG = 1
01041 3210 IF (IUSE(J),EQ-IUSE(J,1)) GO TO 150
01042 3220 IF (J-EO-1 .OR. IUSE(J) .NE. -IUSE(J-1)) GO TO 153
01043 3230 NG = -1
01044 3240 150 JNG = J + NG
01045 3250 IF (EN(JNG,MPT),LT-0.) GO TO 170
01046 3260 IMELT = TEMP(INC,1)
01047 3270 IF (IMELT .EQ. TEMP(INC,2)) GO TO 150
01048 3280 IMELT = TEMP(INC,2)
01049 3290 IF (IMELT .EQ. TEMP(INC,3)) GO TO 157
01050 3300 WRITE (JOUT,106)
01051 3310 156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER )
01052 3320 C JTH SPECIES A SOLID IEM=01, IJ-MELTH SPECIES A LIQUID IEM IS 01
01053 3330 157 IF (ITP-67. TMELT-OR. ITP-AND. TT-EO. TMELT) GO TO 169
01054 3340 IF (ITP-OR. TT-LE. TMELT-150.0) GO TO 1165
01055 3350 JSOL = J
01056 3360 JLIQ = JNG
01057 3370 GO TO 159
01058 3380 C JTH SPECIES A LIQUID IEM=01, IJ-MELTH SPECIES A SOLID IEM IS 01
01059 3390 158 IF (ITP-LT. TMELT-OR. ITP-AND. TT-EO. TMELT) GO TO 169
01060 3400 IF (ITP-OR. TT-GE. TMELT+150.0) GO TO 1165
01061 3410 JSOL = JNG
01062 3420 JLIQ = J
01063 3430 159 TLM = ALOG (TMELT)
01064 3440 TT = TMELT
01065 3450 EN(JNG,MPT) = .5 * EN(JNG,MPT)
01066 3460 EN(J,MPT) = EN(JNG,MPT)
01067 3470 GO TO 165
01068 3480 C WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
01069 3490 1165 EN(J,MPT) = EN (JNG, MPT)
01070 3500 IUSE(J) = -IUSE(J)
01071 3510 IUSE (JNG) = -IUSE (JNG)
01072 3520 EN(JNG,MPT) = 0.

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01132 3530 WRITE(JOUT,16) (SUBJMG,I), I = 1,3) (SUB(J,I), I = 1,3)
01140 3540 FORMAT (10X,22PHASE CHANGE, REPLACE ,3A9.6M WITH ,3A9)
01145 3550 GO TO 40
01146 3560
01150 3570 IF (11.LT.TEMP(INC,1) .AND. TEMP(INC,1) .NE. TLOW) GO TO 169
01152 3580 IF (11.GT.TEMP(INC,2)) GO TO 169
01153 3590 SUM = 0.
01156 3600 DO 167 I = 1,L
01160 3610 SUM = SUM + ALL(J)*X(I)
01161 3620 DELF = MOD(J)-SUM
01166 3630 IF (171) WRITE(JOUT,16) IDELF,SIZEF
01167 3640 IF (171) GO-SUM(I) (J) = E15.7,10X,10PREVIOUS DELTA G = ,E15.7)
01171 3650 IF (171) GO-SIZE .OR. DELF.GE.0. GO TO 169
01172 3660 SIZEF = 0.71F
01173 3670 JDELF = J
01175 3680 IF (171) GO-SUM(I) (J) = E15.7,10X,10PREVIOUS DELTA G = ,E15.7)
01177 3690 IF (171) GO-SIZE .OR. DELF.GE.0. GO TO 169
01201 3700 J = JDELF
01202 3710
01203 3720 WRITE(JOUT,136) (SUB(J,I), I = 1,3)
01211 3730
01212 3740 FORMAT (10X,9HADD ,3A9)
01213 3750 IUSE(J) = - IUSE(J)
01219 3760 CONVG = .FALSE.
01221 3770 JSA = 1
01223 3780 CALL CPMS
01225 3790 TM = MUMB
01227 3800 IF (1.NOT. SHOCK) WRITE(JOUT,77) NPT,X(I), I = 1,1),TM
01230 3810
01231 3820 FORMAT (11,14F9.3)
01232 3830 JSA = 1
01234 3840 IF (171) AND CONVG) CALL CPMS
01235 3850 ITHUMB = 100
01236 3860 GO TO 43
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EOLBRM

DATE 101500

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01271 0090 1 CPRIMPT1,OLVPT1,MPT1,OLVTP1,MPT1,GAMMAS1,MPT1,VL1M1,MPT1
01307 0100 201 FORM1 (7MOP1M1=13.6,3X,4MPCP=E13.6,3X,2MP=E13.6,3X,2HT=E13.6,3X,2M
01307 0110 1M/R=E13.6,3X,4MS/R=E13.6,3X,3MMU=E13.6,3X,5MCP/R=E13.6,3X,6MDLVPY
01310 0120 2=E13.6,3X,6MDLVPY=E13.6,3X,9GAMMA1S1=E13.6,3X,2M1=E13.6)
01310 0130 RETURN
01310 0140 C ERROR, SET 11=0
01311 0150 873 11=0
01312 0160 MPT = MPT-1
01313 0170 RETURN
01314 0180 END

```

END OF COMPIATION: NO DIAGNOSTICS.

AMD6.0 FROZEN

PROZEN

FORM 5 PROZEN.FROZEN
MSA E3 -10/15/80-13:06:33 (10.1)

SUBROUTINE FROZEN ENTRY POINT 000305

STORAGE USED: CODE(1) 000360: DATA(0) 000041: BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 POINTS 000335
0005 SPECIES 017004
0006 MISC 001701
0007 INDX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0010 PMS
0011 AL06
0012 EXP
0013 NEAR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000066	1356	0001	000251	2076	0001	000022	SIL	0001	000050	SSL	0001	000120	60L
0002	000165	ALL	0001	000313	921L	0001	000321	903L	0005	011052	A	0006	000400	AM
0006	000705	AM1	0006	001135	AMUM	0003	000000	ATMM	0006	000004	ATOM	0006	000314	BO
0004	000545	BOP	0007	000036	CALCH	0000	R 000005	CC	0005	000000	COEF	0007	L 000001	CONVG
0004	R 000032	CPR	0004	000706	CPR1	0006	R 000434	CPSUM	0006	000634	DATA	0005	010424	DELM
0006	001560	DEMS	0000	R 000007	DLMT	0004	R 000044	DLVPT	0004	R 000047	DLVTP	0005	R 004312	EM
0005	010150	ENLM	0004	001700	ENLSAV	0006	000000	ENM	0006	001676	ENML	0006	001677	ENSAVE
0006	001414	ENTM	0004	000436	ENRAT	0006	001518	EZ2	0006	001527	FOX	0004	R 000101	BARRAS
0003	000001	GRE1	0007	L 000003	HP	0006	000642	HPP	0006	R 000637	MSUM0	0004	R 000000	MSUM
0005	R 010376	MD	0007	000030	IC	0007	000000	IOE006	0007	000015	IMAT	0000	I 000010	IMC
0000	000015	IMPS	0007	000023	IONS	0007	000021	IP	0007	000037	IOSAVE	0007	000316	IO1
0007	000005	ISV	0007	000034	IT	0005	I 012666	IUSE	0006	I 000004	J	0007	000026	JL10
0007	000025	J50L	0007	I 000031	J51	0007	000014	KMAT	0006	000043	LLMT	0007	000040	LSAVE
0007	000006	MOLES	0006	000707	NAME	0007	I 000029	MC	0007	000022	NEUR	0007	I 000035	MF2
0007	000012	MLM	0007	000017	MOF	0007	000020	MONIT	0007	000007	NP	0007	I 000011	NP1
0007	000027	MRELIC	0007	I 000013	NS	0000	I 000000	MSPP1	0007	000010	NT	0006	000435	OF
0006	001644	ORF	0004	000116	P	0003	000002	PATM	0006	001343	PECUT	0006	R 000633	PP
0004	R 000217	PPP	0003	000003	RBAR	0003	000004	RBR	0006	000444	RM	0006	001611	RHOP
0006	001612	RMV	0000	R 000001	RNV	0006	001476	RTEMP	0003	R 000005	RVR	0005	R 000064	S
0007	003013	SMOCH	0005	014460	SLM	0004	010251	SONVEL	0007	L 000004	SP	0000	R 000006	SS
0004	R 000015	SSUM	0005	015364	SUB	0000	R 000003	SUMH	0006	000001	SUMH	0000	R 000002	SUMS
0006	R 000003	SO	0004	000150	T	0005	R 016514	TEMP	0006	000632	THIGH	0006	R 001643	TLM
0006	R 000030	TLOW	0006	000627	TM	0006	000631	TMI0	0004	R 000320	TOTM	0007	000002	TP
0006	R 000002	TT	0004	R 000266	TTT	0004	000202	V	0004	R 000303	VLM	0006	000496	VMIN
0007	L 700032	VOL	0006	000650	VPLS	0004	R 000234	VM	0006	000652	VP			

PROZEN

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00171 560 GAMASIMP1 = CPSUM/(CPSUM-1./UMINF2)
00172 570 VLR(MPT) = RVRO1/(UMINF210PP)
00173 580 UMINP1 = UMINF2)
00174 590 OLAPT(MPT) = -1.
00175 600 OLATP(MPT) = 1.
00176 610 TOTNIMP1 = TOTNIMP2)
00177 620 PPMIMP1 = PP
00200 630 CPMIMP1 = CPSUM
00201 640 IF (T1.L1.(TLOW-150.1166 TO 903
00203 650 IF INC .EQ. 0) RETURN
00205 660 INC = 0
00206 670 DO 901 J = 1,N5
00208 680 IF (IUSE1(J) .EQ. 0 .OR. IUSE1(J) .EQ. - 10000) GO TO 901
00213 690 INC = INC+1
00214 700 IF (EM1(J,MF2) .LE. 0.0) GO TO 901
00216 710 IF (T1.L1.TEMP1INC,1)-50. .OR. T1.67.TEMP1INC,2)+50.1 GO TO 903
00220 720 901 CONTINUE
00222 730 RETURN
00223 740 903 IF=0.
00224 750 MPT = MPT+1
00225 760 RETURN
00226 770 END

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PROZ0000

END OF COMPILE: NO DIAGNOSTICS.

AM06.P GAMZFF

3F015 GAMEFF, GAMEFF
HSA E3 -10/15/80-13:06:02 (2.)

SUBROUTINE GAMEFF ENTRY POINT 000176

STORAGE USED: CODE(1) 000217; DATA(0) 000000; BLANK COMMON(2) 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 XPRR
0004 SORT
0005 MERR39

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000036 10L 0001 000025 156 0001 000132 20L 0000 R 000002 AMK
0000 R 000006 CFA 0000 R 000005 CGM 0000 R 000001 G 0000 R 000004 GM
0000 I 000000 I 0000 000014 INJPS 0000 R 000003 GP

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00101 1* SUBROUTINE GAMEFF (V,GAMMA,A,M,H)
00102 2* DIMENSION A(13),GAMMA(13),H(13),V(13)
00103 3* C
00104 4* DO 50 I = 2,M
00105 5* G = GAMMA(I)
00110 6* AMK = 1.0
00111 7* IF (G .GT. 1.0) 60 TO 10
00112 8* G = 1.0010
00113 9* GP = G * 1.0
00114 10* IF (GP .GT. 1.0)
00115 11* GM = G - 1.0
00116 12* CGM = SORT(G)*(2.0/GP)+16P/(2.0*GM)
00117 13* CFA = CGM*SORT(2.0*G+1.0 - (1.0/A(I)))+(GM/G)/GM)
00120 14* IF (ABS(V(I)) - CFA) .LE. 5.0E-5) 60 TO 50
00121 15* IF (G .LT. 2.0) 60 TO 20
00122 16* IF (AMK .LT. 0.0) 60 TO 50
00123 17* AMK = -1.0
00124 18* G = GAMMA(I)
00125 19* GO TO 10
00126 20* G = 6 * AMK*(V(I) - CFA)
00127 21* IF (G .GT. 1.0) 60 TO 10
00128 22* IF (AMK .LT. 0.0) 60 TO 50
00129 23* AMK = -1.0
00130 24* G = GAMMA(I)
00131 25* GO TO 10
00132 26* H(I) = G
00133 27* RETURN
00134 28* END

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END OF COMPILATION: NO DIAGNOSTICS.

GAMEFF

3H06,P

GAUSS

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8FOR,S GAUSS,GAUSS
HSA E3 -10/15/68-13:06:54 (7.1)

SUBROUTINE GAUSS ENTRY POINT 000011

STORAGE USED: CODE(1) 000031; DATA(0) 000126; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 DOUBLE 001560
0004 INDEX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0005 MERR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000107	10L	0001	000011	1106	0001	000003	1206	0001	000062	1276	0001	000130	1526	
0001	000161	1676	0001	000204	1176	0001	000115	18L	0001	000256	2106	0001	000267	2136	
0001	000141	22L	0001	000361	23L	0001	000333	2316	0001	000167	31L	0001	000275	45L	
0001	000303	47L	0001	000340	51L	0001	000020	8L	0001	000101	9L	0004	000036	CALCH	
0000	D	COEFF	0004	000001	CONVG	0003	D	000000	6	0004	000003	HP	0000	1	
0004	000030	IC	0004	000000	IOERUG	0000	000071	IMJPS	0004	000023	10MS	0004	000056	I	
0004	000037	IOSAVE	0004	000016	101	0004	000005	ISV	0004	000034	IT	0004	000021	IP	
0000	I	000054	IUSE1	0000	I	000037	J	0004	000025	J50L	0004	000031	J51		
0000	I	000061	K	0004	000014	KMAT	0004	000040	LSAVE	0004	000006	MOLES	0004	000024	NC
0004	000022	NEUR	0004	000035	NFZ	0004	000012	NLM	0000	I	000058	NN	0004	000017	NOF
0004	000020	NOMIT	0004	000007	NP	0004	000011	NPT	0004	000027	NREAC	0004	000013	MS	
0004	000010	NT	0004	000033	SHOCK	0004	000004	SP	0000	D	000050	SUM	0000	R	000060
0004	000002	TP	0004	000032	VOL	0004	000032	VOL	0003	D	001510	X	0000	D	000052

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00101	10	SUBROUTINE GAUSS	000000
00103	20	COMMON/DOUBLE/6120,211,X120)	000000
00104	30	COMMON /INDEX/ IOERUG,CONVG,TP,NP,SP,ISV,MOLES,NB,NT,NPT,NLM,NS, /INDEX/	000000
00104	40	KMAT,IUSE,IOI,NOMIT,IP,NEUR,IONS,NC,J50L,JL10, /INDEX/	000000
00104	50	NREAC,IC,J51,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE /INDEX/	000000
00105	60	DOUBLE PRECISION COEFF1207,6,SUM,X,Z	000000
00105	70	BEGIN ELIMINATION OF NINTH VARIABLE	000000
00106	80	IUSE1:IUSE+1	000000
00107	90	DO 45 NN = 1,IUSE	000002
00112	100	IF (NN.NE. IUSE1) GO TO 8	000011
00114	110	:7 (G(NN,NN)) 31,23,31	000014
00114	120	SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW	000014
00117	130	DO 10 I=NN,IUSE	000020
00122	140	COEFF(I) = 1.OE38	000007
00123	150	IF (G(I,NN).EQ.O.) GO TO 10	000051
00125	160	COEFF(I) = 0.	000054
00126	170	DO 10 J=NN,IUSE1	000062

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00131 180 SUM = G(I,J)
00132 190 IF (SUM.LT.O.) SUM=-SUM
00133 200 IF (J.NE.MN) GO TO 9
00134 210 Z = SUM
00135 220 GO TO 10
00136 230 9 IF (SUM.GT.COEFX(I)) COEFX(I)=SUM
00137 240 10 CONTINUE
00138 250 COEFX(I) = COEFX(I)/Z
00139 260 10 CONTINUE
00140 270 TEMP = 1.OE10
00141 280 I=0
00142 290 DO 22 J = MN,IUSE
00143 300 IF (COEFX(J).GE. TEMP) GO TO 22
00144 310 TEMP = COEFX(J)
00145 320 I=J
00146 330 22 CONTINUE
00147 340 INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE MNTH
00148 350 VARIABLE FROM THE REMAINING EQUATIONS
00149 360 C INTERCHANGE EQUATIONS I AND MN
00150 370 IF (MN.EQ.1) GO TO 31
00151 380 DO 30 J = MN,IUSE1
00152 390 Z=G(I,J)
00153 400 G(I,J)=G(MN,J)
00154 410 G(MN,J)=Z
00155 420 30 G(MN,J) = Z
00156 430 C DIVIDE MNTH ROW BY MNTH DIAGONAL ELEMENT AND ELIMINATE THE MNTH
00157 440 VARIABLE FROM THE REMAINING EQUATIONS
00158 450 31 K = MN + 1
00159 460 DO 36 J = K, IUSE1
00160 470 IF (G(MN,MN).EQ.Q) GO TO 23
00161 480 36 G(MN,J) = G(MN,J)/G(MN,MN)
00162 490 IF (K.EQ. IUSE1) GO TO 45
00163 500 DO 44 I = K, IUSE1
00164 510 DO 44 J = K, IUSE1
00165 520 G(I,J) = G(I,J) - G(I,MN)*G(MN,J)
00166 530 44 CONTINUE
00167 540 C BACKSOLVE FOR THE VARIABLES
00168 550 K = IUSE1
00169 560 47 J = K + 1
00170 570 X(K) = 0.O00
00171 580 SUM = 0.O
00172 590 IF (IUSE1.LT. J) GO TO 51
00173 600 DO 50 I = J, IUSE1
00174 610 SUM = SUM + G(I,X(I))
00175 620 51 X(K) = G(MN,IUSE1) - SUM
00176 630 K = K - 1
00177 640 IF (K.NE. 0) GO TO 47
00178 650 RETURN
00179 660 23 IUSE = IUSE-1
00180 670 RETURN
00181 680 END

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ORIGINAL PAGE IS
OF POOR QUALITY

GAUSS

SHDG, P

WCALC

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MCALC

FOR S MCALC-MCALC
MSA E3 -10/15/80-13:06:58 (11,1)

SUBROUTINE MCALC ENTRY POINT 000526

STORAGE USED: CODE(1) 000542; DATA(0) 000066; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 00000A
0004 HOLCON 000010
0005 POINTS 000101
0006 SPECES 017106
0007 MISC 001701
0010 INDI 000041
0011 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0012 CPHS
0013 ALG
0014 MUDUS
0015 NIOZS
0016 MERRIS

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STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000070	1436	0001	000107	15L	000131	16L	0001	000138	18G	0001	000139	172F	
0001	000162	1776	0001	000204	2106	0001	000275	2276	0001	000170	30L	0001	000026	4L
0001	000177	50L	0001	000432	500L	0001	000251	55L	0001	000265	56L	0001	000307	70L
0001	000467	75L	0000	000010	76F	0001	000477	80L	0000	000024	85F	0001	000037	9L
0001	000312	90L	0006	R 011032	A	0004	J 000001	AG	0007	J 000490	AM	0007	R 000705	AM1
0000	R 000002	AMW	0007	R 001135	AMW	0003	000000	ATM	0007	000004	ATOM	0004	I 000000	BLV
0007	000314	80	0007	000545	80P	0010	L 000036	CALCH	0006	000000	COEF	0010	000001	COMVG
0005	000032	CP8	0007	R 00706	CP81	0007	R 000634	CPSUM	0007	R 000634	DATA	0006	010624	DCLM
0011	000002	DEMAND	0007	001560	DEMS	0005	000064	DLVPT	0005	00007	DLVTP	0006	R 004312	EN
0004	000000	END	0000	R 000007	ENJ	0006	010150	EMLN	0007	001700	EMLSAV	0007	000000	ENM
0007	001376	ENML	0007	001677	ENSAVE	0007	R 001414	ENTH	0007	000636	EGRAT	0007	I 001445	FAZ
0007	I 001327	FOX	0003	000001	GMEY	0011	000000	GRAPH	0010	000003	HP	0007	R 000642	HPP
0007	R 000037	HSUBG	0005	000000	MSUM	0006	R 010376	HO	0000	I 000005	I	0010	000030	IC
0010	000000	IOEBUG	0004	000002	IE	0010	000015	IMAT	0000	000044	INJPS	0010	000023	IONS
0010	000021	IP	0010	000037	IOSAVE	0010	000016	IOI	0000	I 000006	IS	0010	000005	ISV
0010	000034	IT	0006	I 016266	IUSE	0004	I 000003	IZERO	0000	I 000031	J	0010	000026	JL10
0011	I 000001	JOUT	0010	000025	JSOL	0000	I 000004	K	0010	000014	KMAT	0010	I 000012	L
0007	I 000463	LLMT	0010	000040	LSAVE	0004	000005	MOL	0010	L 000006	MOLES	0000	I 000003	M
0007	I 000707	NAME	0010	000024	MC	0010	000022	MEWR	0010	000035	MF2	0010	000017	MOF
0010	000020	MOMIT	0010	000007	MP	0010	I 000011	NPT	0010	I 000027	MREAC	0010	I 000013	MS
0000	I 000000	MSPP1	0010	000010	MY	0007	I 001135	MUM	0007	R 000635	OF	0004	I 000006	OF
0007	001644	OXF	0003	000002	PATM	0007	R 001363	PECVT	0007	R 000633	PP	0003	R 000003	R8AP
0003	000004	R8R	0007	000644	RH	0007	001611	RHOP	0007	R 001612	RHW	0007	R 001476	RTEPP
0003	000005	R8R	0006	R 004064	S	0010	L 000033	SHNCH	0006	016460	SLM	0010	000004	SP
0005	R 000015	SSUM	0006	015364	SUB	0007	000001	SUMN	0007	000003	SD	0006	R 016514	TFMD

0007 R 000632 THIGH 0007 R 001643 TLM 0007 R 000630 TLOW 0007 R 000627 TM 0007 000631 THID
 0010 000002 TP 0000 R 000001 TSAVE 0007 R 000002 TT 0007 000646 VMIN 0010 L 000032 VOL
 0007 000650 VPLS 0007 R 000652 VP 0004 000007 ZERO

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00101 10 SUBROUTINE HCALC
00102 20 CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS
00103 30 COMMON /CONSS/ AMN,GET,PATM,ROAR,ROR,RVR
00104 40 COMMON /MOLCOM/ EMO,AG,IE,ITERO,BLK,MOL,OK,ZERO
00105 50 COMMON/OOINTS/MSUM(13),SSUM(13),CPR(13),OLVPT(13),OLVPT(13)
00106 60 COMMON/SPECFS/COEF(12),T(150),S(150),EM(150),13 ENLM(150),MO(150)
00107 70 1 .DELN(150),A(15,150),SUB(150,3),TUSE(150),TEMP(150,2),SLM(150)
00108 80 INCLUDE SPECPR
00109 90 COMMON /MISC/ ENN,SUMM,TT,SD,ATOM(3,101),LLMT(25),BO(25),
00110 100 BO(25,2),TM,TLOW,THID,THIGH,PP,CP,SUM,OF,EGRAT,
00111 110 MSUBO,AM(2),MP(2),RM(2),VM(2),VPLS(2),UP(2),
00112 120 DA,A(25),AM1,CPR1,NAME(25,6),AMU(25,6),PECUT(25),
00113 130 ENM(25),FAZI(25),TEMP(25),FOX(25),DEMS(25),RMOF,
00114 140 MMU(25),TLN,OXF(26),EMM,ENSAVE,CALSAV
00115 150 COMMON /INDX/ IOEBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,MT,NPT,L,MS,
00116 160 MWAT,IMAT,IOI,MOF,NOMIT,IP,NEUR,TOMS,NC,JSL,JLTO,
00117 170 MREAC,IC,LVOL,SHOCK,11,MFZ,CALCH,IOSAVE,LSAVE
00118 180
00119 190 COMMON /CCC/ GRAPH,JOUT,DEMAND
00120 200
00121 210 DIMENSION NUM(25,6)
00122 220 EQUIVALENCE (AMU,NUM)
00123 230 INTEGER AG,BLK,FAZ,FOX,OX
00124 240 LOGICAL CALCH,MOLES,SHOCK,VOL
00125 250 TSAVE = TT
00126 260 IF (AM(1) .GT. 0.0 .AND. AM(2) .GT. 0.0) GO TO 4
00127 270 AM1 = AM(2)
00128 280 IF (AM(2) .LE. 0.0) AM1 = AM(1)
00129 290 GO TO 9
00130 300 4 AM1 = (OF+1.1*AM(1)+AM(2))/(AM(1)+OF+AM(2))
00131 310 9 TM = 0.
00132 320 IF (PP.GT.0.1) TM = ALOG(PP+AM1)
00133 330 SSUM(MPT) = 0.
00134 340 MPP(1) = C.
00135 350 MPP(2) = 0.
00136 360 MSUBO = 0.
00137 370 CPR1 = 0.
00138 380 AMN = 11.0F1
00139 390 C LOOP ON REACTANTS. IF OXIDANT, K = 1, IF FUEL, K = 2.
00140 400 DO 900 M=1,MREAC
00141 410 K=2
00142 420 IF (FOX(M).EQ.OX) K=1
00143 430 IF (NAME(M,6).NE.IZERO) GO TO 90
00144 440 IF (NOT-CALCH) GO TO 15
00145 450 TT = RTEMP(M)
00146 460 C IS TT IN RANGE
00147 470 15 IF (SMOCH) GO TO 16
00148 480 IF (TT .LT. TLOW - 100.0 .OR. TT .GT. THIGH + 1000.0) GO TO 75
00149 490 16 J=NUM(M,6)
    
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MCALC

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00162 500 IF (J.NE.C) 60 TO 90
00164 510 DO 10 J=1,N
00167 520 DATA(J) = 0.0
00171 530 DO 30 I=1,5
00174 540 IF (AMUMIN,I) .LE. 0.0) 60 TO 50
00176 550 DO 20 J=1,N
00201 560 IF (LLMT(I).EQ. NAMEIN,I) 60 TO 30
00204 570 DATA(J) = DATA(J) + AMUMIN,I)
00206 580 IS=0
00207 590 DO 70 J=1,NS
00212 600 IF (IUSE(J).EQ.0) 60 TO 55
00214 610 IS = IS+1
00215 620 IF (FAZIN).EQ.0) 60 TO 70
00217 630 IF (TT.GT. TEMP(15,2).AND. TEMP(15,2).NE. THIGH) 60 TO 70
00221 640 IF (TT.LT. TEMP(15,1).AND. TEMP(15,1).NE. TLOW) 60 TO 70
00223 650 GO TO 56
00224 660 55 IF (FAZIN).NE. AG.AND. FAZIN).NE. BLN) 60 TO 70
00226 670 56 DO 60 I=1,N
00231 680 60 IF (A(I,J) .NE. DATA(I)) 60 TO 70
00234 690 NUMIN,6) = J
00235 700 GO TO 90
00236 710 70 CONTINUE
00240 720 GO TO 80
00241 730 90 IF (MOLES) ENJ = PECUMIN/MP(M)
00243 740 IF (I.NOT.MOLES) ENJ = PECUMIN/RMUMIN)
00245 750 ENJ = ENJ/AMN
00246 760 IF (K.EQ.1) ENJ = ENJ*OF
00250 770 IF (NAMEIN,6).NE. IZERO) 60 TO 500
00252 780 I = NS
00253 790 NS = J
00254 800 TLM = ALOG(17)
00255 810 IF (I.NOT.CALCH) ENJ,MPT) = ENJ
00257 820 CALL CPHS
00260 830 NS = I
00261 840 IF (MO(J).GT. -.01 .AND. MO(J).LT. .01) MO(J) = 0.
00263 850 RT(MP(M) = IT
00264 860 IF (VOL) MO(J)=MO(J)-1.
00266 870 ENTHIN) = RBAR*TT*MO(J)
00267 880 CPRI = CPRI + CPSUM
00270 890 500 MSUBO = MSUBO + ENTHIN)*ENJ
00271 900 HPPR) = HPPR + ENTHIN)*ENJ
00272 910 900 SSUM(MPT) = SSUM(MPT) + ENJ*(LS(J) - ALOG(ENJ) - TM)
00274 920 TT = TSAVE
00275 930 MSUBO = MSUBO/RBAR
00276 940 RETURN
00277 950 75 WRITE(JOUT,76)
00301 960 76 FORMAT (1/20X,5HREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA
00302 970 11M MCALC/)
00303 980 RETURN
00304 990 80 WRITE(JOUT,85) N
00307 1000 85 FORMAT (1/20X,12,42MH REACTANT IS NOT IN THERMO DATA IN MCALC/)
00310 1010 RETURN
00310 1020 END

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END OF COMPILATION: NO DIAGNOSTICS.

MCALC

DATE 101500

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ANDG.P

LISTIT

SPRT.S LISTIT
FUMPUA 201111 10/15/80 13:07:03

LISTIT

SEVIGNIN200+TPP(10)-LISTIT
 1 AFOR,S LEVIS,BLOCK1,LEVIS,BLOCK1
 2 AFOR,S LEVIS,CPMS,LEVIS,CPMS
 3 AFOR,S LEVIS,DETON,LEVIS,DETON
 4 AFOR,S LEVIS,FOLDM,LEVIS,FOLDM
 5 AFOR,S LEVIS,FROZEN,LEVIS,FROZEN
 6 AFOR,S LEVIS,GAMEFF,LEVIS,GAMEFF
 7 AFOR,S LEVIS,GAUSS,LEVIS,GAUSS
 8 AFOR,S LEVIS,MCALC,LEVIS,MCALC
 9 AFOR,S LEVIS,LTCPS,LEVIS,LTCPS
 10 AFOR,S LEVIS,MAIN,LEVIS,MAIN
 11 AFOR,S LEVIS,MATRIX,LEVIS,MATRIX
 12 AFOR,S LEVIS,OUT1,LEVIS,OUT1
 13 AFOR,S LEVIS,REACT,LEVIS,REACT
 14 AFOR,S LEVIS,RMTOUT,LEVIS,RMTOUT
 15 AFOR,S LEVIS,ROCKET,LEVIS,ROCKET
 16 AFOR,S LEVIS,RREAD,LEVIS,RREAD
 17 AFOR,S LEVIS,SAVE,LEVIS,SAVE
 18 AFOR,S LEVIS,SEARCH,LEVIS,SEARCH
 19 AFOR,S LEVIS,SMCK,LEVIS,SMCK
 20 AFOR,S LEVIS,THERMP,LEVIS,THERMP
 21 AFOR,S LEVIS,VARFMT,LEVIS,VARFMT
 22 ABREPT PRINTB

ANDG.P LTCPS

ORIGINAL PAGE IS
 OF POOR QUALITY

AFOR,S LTCPS,LTCPS
MSA E3 -10/15/80-13:07:03 (2.)

SUBROUTINE LTCPS ENTRY POINT 000205

STORAGE USED: CODE(1) 000221; DATA(1) 000130; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000004
0004 LOWTH 001201

EXTERNAL REFERENCES (BLOCK, NAME)

0005 PASS1
0006 CHR512
0007 GOUT
0010 RDATA1
0011 ROCHAR
0012 MDCODS
0013 RDATAF
0014 MIO15
0015 MIO25
0016 MERR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000006 10L 0000 000072 100F 0001 000025 1246 0001 000045 1326 0001 000111 1446
0001 000113 1476 0001 000124 1566 0001 000026 20L 0001 000051 30L 0001 000122 46L
0003 000000 ATMM 0004 R 000361 CPL 0003 000001 GHET 0004 R 000551 HL 0000 000056 1
0004 000113 ILSP 0000 000024 IMN 0000 000107 INJPS 0000 000000 INLTHN 0000 000012 ISMMN
0000 000015 ITMPMN 0000 000067 J 0000 000071 K 0000 000000 MLISP 0000 000070 MT
0003 000002 PATM 0003 R 000073 RBAR 0003 000004 RBR 0003 000062 RDUM 0003 000005 RVR
0004 R 000074 SL 0004 R 000001 SUBLT 0004 R 000171 TL

SUBROUTINE LTCPS		LTCP 10	
00101	10 C		000000
00101	20 C		000000
00101	30 C	PROCESS LOW TEMPERATURE CP,M,S (VIA MIPS I/O)	000000
00101	40 C		000000
00101	50 C	DIMENSION MIPS OUTPUT ARRAYS	000000
00103	60 C	DIMENSION INLTHN(10), ISMMN(13), ITMPMN(7), IMN(5,6), RDUM(4)	000000
00103	70 C		000000
00104	80 C	COMMON /CONSTS/ ATMM, GHET, PATH, RBAR, RBR, RVR	000000
00105	90 C	COMMON /LOWTH/ MLTSP, SUBLT(40,3), TL(40,3), CPL(40,3), HL(40,3),	000000
00105	100 C	SL(40,3), ILSP(40)	000000
00105	110 C		000000
00105	120 C	SET DATA FOR MIPS OUTPUT	000000
00106	130 C	DATA INLTHN/24HTYPE THE NUMBER OF LOW T,	000000
00106	140 C	1 SAME TEMPERATURE SPECIES TO BE ENTERED /	000000

LTCMNS

```

00110 150 DATA ISMNH/10MTYPE SPECIES NAME /
00112 160 DATA ITHMNH/2MTYPE NUMBER OF TEMPERATURES, THIS SPECIES/
00114 170 DATA IMH/3MTYPE TL CPL ML, SL WHERE -
00116 180 36M TL-TEMPERATURE
00118 190 36M CPL-CONSTANT PRESSURE SPECIFIC HEAT,
00120 200 36M ML-ENTHALPY
00122 210 36M SL-ENTROPY
00124 220
00126 230
00128 240
00130 250
00132 260
00134 270
00136 280
00138 290
00140 300
00142 310
00144 320
00146 330
00148 340
00150 350
00152 360
00154 370
00156 380
00158 390
00160 400
00162 410
00164 420
00166 430
00168 440
00170 450
00172 460
00174 470
00176 480
00178 490
00180 500
00182 510
00184 520
00186 530
00188 540
00190 550
00192 560
00194 570
00196 580
00198 590
00200 600
00202 610
00204 620
00206 630
00208 640
00210 650
00212 660

DATA ISMNH/10MTYPE SPECIES NAME /
DATA ITHMNH/2MTYPE NUMBER OF TEMPERATURES, THIS SPECIES/
DATA IMH/3MTYPE TL CPL ML, SL WHERE -
36M TL-TEMPERATURE
36M CPL-CONSTANT PRESSURE SPECIFIC HEAT,
36M ML-ENTHALPY
36M SL-ENTROPY

MLTSP=0
CALL PAGIT
CALL CHRSLZ13,
CALL GOUTINLTM,561
CALL RDATA,11,MLTSP,5101

LOOP FOR EACH SPECIES
DO 60 I=1,MLTSP
CALL GOUT,ISMNH,17)
CALL ROCMLR,ROUM,2,-1,520)
DECODE(100,ROUM) (SUBLT(I,J),J=1,3)
CALL GOUT,ISMNH,92)
CALL RDATA(1,ML,530)
IFML LT 1 .OR. MT.GT.3) GO TO 30
ILSP,11=0

LOOP FOR EACH TEMPERATURE
DO 50 K=1,MT
DO 45 J=1,5
CALL GOUT,ISMNH,11,36)
CONTINUE
CONTINUE
DO 40 J=1,4
ROUM,11=0.
CONTINUE
CALL RDATA(1,ROUM,504)
TL(I,1)=ROUM(1)
CPL(I,1)=ROUM(12)
ML(I,1)=ROUM(13)
SL(I,1)=ROUM(14)
ILSP(11)=ILSP(11)+1
CPL(I,1)=CPL(I,1)/ROUM
ML(I,1)=ML(I,1)/TL(I,1)*ROUM
SL(I,1)=SL(I,1)/ROUM
CONTINUE

END SPECIES LOOP
CONTINUE

RETURN
FORMAT(340)
END

```


DATE 101500

LYCPMS

2ND6,P RAIN

MAIN

AFON.S MAIN.MAIN
MSA C3 -10/15/00-13:07:06 (39.)

MAIN PROGRAM

STORAGE USED: CODE(1) 001510; DATA(1) 000720; BLANK COMP(12) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCOM 000010
0005 POINTS 000335
0006 SPECS 017106
0007 WISC 001701
0010 INDI 000041
0011 PERI 000166
0012 CCC 000003
0013 CEUEL 000004
0014 WIM2 000002

EXTERNAL REFERENCES (BLOCK, NAME)

0015 RATES
0016 MPSTMT
0017 PAGE1
0020 CMRSIZ
0021 GOUT
0022 RDATAI
0023 RNCAD
0024 COALCY
0025 LTCPS
0026 RDCMAR
0027 WDCOOR
0030 NOVAB3
0031 HOLG17
0032 REACT
0033 SEARCH
0034 THERMP
0035 DETON
0036 RCHREI
0037 SMCR
0038 MPSTEN
0041 NIMTPS
0042 WUDUS
0043 W1025
0044 WCR26
0045 WREMS
0046 WIDUS
0047 W1036
0050 W1016
0051 WML6
0052 WML6
0053 WVEFS
0054 AL06
0055 WSTOP6

MAIN

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000530	10F	0001	000406	100L	0001	000233	11L	0001	000601	11211L	0001	000536	1211L
0001	000574	1212L	0001	000733	1215L	0001	000733	1215L	0001	000237	15L	0001	000021	154R
0001	000414	181L	0001	000057	21L	0000	000337	203L	0001	000076	203L	0001	000444	205L
0001	000452	206L	0000	000577	207F	0001	000505	208L	0000	000548	21F	0001	000313	210L
0001	000655	211F	0001	000762	213L	0001	000777	214L	0001	000633	215L	0000	000551	22F
0001	000403	25L	0001	000150	3L	0001	001446	301L	0001	001450	302L	0001	001046	304L
0001	0001122	307L	0001	001104	322L	0001	001153	323L	0001	000367	3276	0001	001211	333L
0001	000437	352G	0001	000471	367G	0001	000243	39L	0000	000377	400F	0001	000540	4156
0001	001363	432L	0000	000526	5F	0001	000706	5176	0001	000714	5226	0001	000740	5326
0001	000756	546G	0001	001014	5716	0001	001050	5106	0001	001104	6256	0001	001130	6406
0001	001267	7076	0001	001126	722L	0000	000637	724F	0001	001131	7246	0001	001217	745L
0001	001049	746L	0001	001254	746L	0001	001301	748L	0001	001416	7516	0001	001430	7565
0001	001452	790L	0001	001462	791L	0001	001476	800L	0001	000246	90L	0001	000277	97L
0006	R 011052	A	0001	000150	AEAT	0007	000640	AM	0001	000705	AM1	0007	001135	ANUM
0011	000133	APP	0003	R 000000	ATNM	0007	000004	ATOM	0004	I 000004	BLANK	0007	000514	80
0007	R 000535	BPR	0010	L 000036	CALCH	0007	000000	CE	0000	000000	CDEF	0010	000001	CONVG
0005	000032	CPR	0007	000706	CP21	0007	000634	CPSUM	0007	I 000654	DATA	0006	010624	DELM
0012	000002	DEMAND	0007	001580	DENS	0000	L 000244	DETM	0008	000064	DLVPT	0005	000047	DLVTP
0004	R 000312	EM	0009	I 000000	END	0006	R 010150	ENLM	0007	001700	ENLSAV	0007	R 000000	ENL
0007	R 001676	ENML	0007	001677	ENSAVE	0006	I 010624	ENSMRT	0007	01414	ENTH	0011	L 000045	EOL
0007	R 000636	EQRAY	0000	L 000245	ERRAYO	0000	L 000246	FA	0007	001445	FAZ	0000	L 000257	FIRST
0007	001527	FOX	0000	L 000247	FPECT	0005	000101	GAMMAS	0004	000001	GAS	0003	000001	GNET
0012	000000	GRAPH	0003	000012	J	0010	L 000003	HP	0007	000642	HPP	0007	000637	HSUBD
0005	000000	HSUM	0006	000002	IE	0000	I 000231	I	0010	000030	IC	0000	I 000262	ICARD
0010	I 000000	IOCBUG	0004	I 000002	IE	0010	000015	IMAT	0000	I 000260	IMAM	0000	000265	IMPT2
0000	I 000232	INSERT	0010	L 000023	IONS	0010	000021	IP	0010	000037	IOSAVE	0010	I 000016	IQ1
0000	I 000264	IST	0010	000005	ISV	0010	I 000034	IT	0006	I 016266	IUSE	0004	I 000003	I2
0000	I 000263	J	0010	000026	JL10	0012	L 000001	JOUT	0010	000025	J50L	0010	000031	J51
0010	000014	KMAT	0010	I 000012	L	0007	I 000463	LLMT	0010	000040	LSAVE	0000	I 000233	M17
0007	R 001644	MIX	0000	I 000235	MLOW	0000	L 000250	MHMG	0004	000005	MOL	0010	L 000006	MOLES
0007	I 000707	NAME	0010	I 000024	NC	0000	I 000236	MCD	0010	L 000022	NEWR	0010	000035	NF2
0000	I 000234	NMLT	0010	I 000017	NOF	0010	I 000020	NOMIT	0000	I 000003	NOMTS	0010	I 000007	NP
0010	000011	NPT	0010	I 000027	NREAC	0010	I 000013	MS	0000	I 000261	MSERT	0000	I 000000	MSPP1
0000	L 000251	NSOM	0010	I 000010	NI	0014	I 000000	NL	0014	L 000001	N2	0007	L 000038	OF
0006	I 010150	OMIT	0004	000006	OX	0007	R 001644	OXF	0007	R 000735	OXFL	0005	R 000116	P
0003	R 000002	PATM	0011	000000	PCP	0007	001363	PECMT	0013	R 000003	PEM	0007	000633	PP
0005	000217	PPP	0000	L 000252	PSIA	0003	R 000003	RBAR	0003	000004	RBR	0000	R 000282	ROUM
0015	L 000000	ROYES	0000	I 000001	REAC	0007	000644	RH	0007	R 001611	RMOP	0000	L 000253	RMT
0007	001612	RNV	0007	001476	RTEMP	0003	000005	RVR	0006	004064	S	0010	L 000033	SMOCK
0006	016640	SLN	0007	R 000003	SO	0005	000251	SOMVEL	0010	L 000008	SP	0011	000047	SPIM
0005	000015	SSUM	0006	I 015364	SUB	0011	000101	SUBAR	0007	R 000001	SUMN	0011	000116	SUPAR
0000	L 000254	SV	0007	R 000003	SO	0005	R 000150	T	0006	016514	TEMP	0007	R 000632	THIGH
0000	I 000002	THRM	0007	001443	TLN	0007	R 000630	TLOW	0007	000627	TM	0007	R 000631	TMID
0005	000320	TOTM	0010	L 000002	TP	0007	000002	TT	0005	000266	TTT	0000	L 000255	TV
0000	L 000256	UV	0005	R 000202	V	0011	000064	VACT	0005	000303	VLM	0007	R 000646	VMIN
0011	000032	VMOC	0010	L 000032	VOL	0007	R 000650	VPLS	0013	000002	VCR	0005	000234	WM
0007	R 000652	VP	0004	000007	ZERO									

000000
000000
000000

MAIN0002
/CONSTS/

COMMON /CONSTS/ ATNM, GNET, PATM, RBAR, RRR, RVR

00100 1* C MAIN PROGRAM
00100 2* C
00101 3*

MAIN

```

00103 COMMON /MOLCON/ EMD,GAS,IE,I2,BLANK,MOL,OX,ZERO 000001
00104 COMMON/POINTS/MSUM(13),SSUM(13),CPRI(13),DLVTP(13),DLVPT(13) 000001
00105 1 .GAMMAS(13),P(126),Y(126),V(13),PP(13),MM(13),SOMVEL(13),YTT(13), 000001
00106 2 .VLM(13),TOTN(13) 000001
00107 COMMON/SPECIES/COEF(12,7,150),S(150),EM(150,13),ENLM(150),MO(150) 000001
00108 1 .DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLN(150) 000001
00109 INCLUDE SPECPR 000001
00110 COMMON /MISC/ EMD,SUM,TT,SP,ATOM(3,101),LLMT(25),BO(25), 000001
00111 BOPI(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EGRAT, 000001
00112 MSUBO,AM(2),MP(2),RH(2),VM(2),VPLS(2),MP(2), 000001
00113 DATA(25),AM1,CPRI,NAME(25,6),ANUM(25,6),PECUT(25), 000001
00114 ENTH(25),FAZ(25),RTEMP(25),FOX(25),DENSI(25),RHOP, 000001
00115 RMV(25),TLN,OF(26),ENML,EMSAVE,ENLSAV 000001
00116 COMMON /INDX/ IDEBUG,CONVG,IP,MP,SP,ISV,MOLES,MP,MT,MPT,L,MS, 000001
00117 KMAT,IMAT,IQI,MOF,NOMIT,IP,NEUR,ION,NC,J,SOL,JL IQ, 000001
00118 REAC,IC,JSI,VOL,SHOCK,IT,MFZ,CALCM,IOSAVE,LSAVE 000001
00119 PCPI(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13), 000001
00120 SUPER(13),APR(13),AEAT(13),EOL 000001
00121 COMMON /CCC/ GRAPH,JOUT,DEMAND 000001
00122 COMMON /CFUEL/CF,MHVV,UCR,PER 000001
00123 COMMON /MIX2/M1,M2 000001
00124 INTEGER BLANK,DATA,END,INSERT,OMIT,REAC,SUB,THRM 000001
00125 DIMENSION NMOTS(150) 000001
00126 DATA (NMOTS(I),I=1,150) 000001
00127 X*AL(5,1) .,ALIL(1) ., ., ., 000001
00128 X*ALCL(2) ., .,ALM(1,5) ., ., ., 000001
00129 X*ALM ., ., .,C ., ., ., ., 000001
00130 X*CS ., ., .,Cn ., ., ., ., 000001
00131 X*M20(1,5) ., ., ., ., ., ., ., 000001
00132 X*O3 ., ., .,SI ., ., ., ., ., 000001
00133 X*SIC ., ., .,SIC2 ., ., ., ., ., 000001
00134 X*SI(5,1) ., ., .,SIL(1,1) ., ., ., ., ., 000001
00135 X*SICL(2) ., ., .,SICL(2,2) ., ., ., ., ., 000001
00136 X*SICL(3) ., ., .,SICL(3,4) ., ., ., ., ., 000001
00137 X*SIM ., ., .,SIM4 ., ., ., ., ., 000001
00138 X*SIM ., ., .,SI2 ., ., ., ., ., 000001
00139 X*SI20 ., ., .,SI2M ., ., ., ., ., 000001
00140 X*SI3 ., ., ., ., ., ., ., ., 000001
00141 DATA INSERT,MII,MMLT,REAC,THRM/MINSE,OMIT,MMNAME,MMREAC,MMTHER/ 000001
00142 DATA MLOW/MHLOW / 000001
00143 DIMENSION ENSERT(3,3),MCD(4),OMIT(3,3) 000001
00144 DIMENSION RNUM(2) 000001
00145 EQUIVALENCE (DELM,ENSERT),(ENLN,OMIT),(MIX,OXF),(OF,OXFL),ISD,SO) 000001
00146 LOGICAL CALCM,DETN,COL,ERATIO,FA,FPCT,MP,IONS,MMHG,MOLES,NEUR, 000001
00147 1 NSQM,OF,PSIA,PMI,SMOCH,SP,SV,TP,JV,UV,VOL 000001
00148 LOGICAL ROYES,FIRST 000001
00149 REAL MIX(26) 000001
00150 NAMELIST /INPT2/ DETN,ERATIO,FA,FPCT,MP,IDEBUG,IONS,MIX,MMHG,NSQM, /INPT2/ 000001
00151 OF,P,PSIA,PMI,SO,SMOCH,SO,SP,SV,T,TP,TV,UV,V 000001
00152 DATA INAM/IN/ 000001

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MAIN

```
00182 600 FIRST=TRUE.
00183 610 CALL MPSINT
00184 620 CF=-1.0
00185 630 N1=0
00186 640 N2=0
00187 650 1 WRITE(JOUT,400)
00188 660 1 00 300 1=1.86
00189 670 MIX(1)=0.8
00190 680 P(1)=0.
00191 690 T(1)=0.
00192 700 300 MIX=0.0
00193 710 TP=.FALSE.
00194 720 HP=.TRUE.
00195 730 TV=.FALSE.
00196 740 UV=.FALSE.
00197 750 SV=.FALSE.
00198 760 REL=.FALSE.
00199 770 SO=0.0
00200 780 SP=.FALSE.
00201 790 SHOCK=.FALSE.
00202 800 DETN=.FALSE.
00203 810 MMWG=.FALSE.
00204 820 PSA=.TRUE.
00205 830 NSQM=.FALSE.
00206 840 IOMS=.FALSE.
00207 850 IDERUG=0
00208 860 FA=.FALSE.
00209 870 OF=.TRUE.
00210 880 ERATIO=.FALSE.
00211 890 FPC=.FALSE.
00212 900 EOL=.TRUE.
00213 910 MEMR=.FALSE.
00214 920 400 FORMAT(1H1)
00215 930 2 CONTINUE
00216 940 MREIC=0
00217 950 NSERT=0
00218 960 NOMIT=0
00219 970 CALL PAGIT
00220 980 JOUT=6
00221 990 IF IRDYES(1) TYPE YES FOR PRINT TO PRINT FILE(35) JOUT=31
00222 1000 CONTINUE
00223 1010 CALL PAGIT
00224 1020 CALL CHR2(1)
00225 1030 CALL GOUT('LEWIS CHEMICAL EQUILIBRIUM PROGRAM',34)
00226 1040 CALL GOUT('1)
00227 1050 CALL GOUT('1)
00228 1060 CALL GOUT('1)
00229 1070 CALL GOUT('1)
00230 1080 CALL GOUT('1 - INSERT THERMODYNAMICS DATA',31)
00231 1090 CALL GOUT('2 - INSERT LOW TEMP EXTENSION THERMO DATA',42)
00232 1100 CALL GOUT('3 - INSERT OR EDIT REACTANTS',29)
00233 1110 CALL GOUT('4 - OMIT SPECIES FROM THERMO DATA',34)
00234 1120 CALL GOUT('5 - INSERT CONDENSED SPECIES',29)
00235 1130 CALL GOUT('6 - INSERT OR EDIT NAMELIST',28)
00236 1140 CALL GOUT('7 - START PROGRAM CALCULATION',30)
00237 1150 CALL GOUT('8 - INSERT OR EDIT COAL DATA',29)
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00361 172* CALL GOUTI TYPE SPECIES TO OMIT FROM THERMO DATA',37)
00362 173* CONTINUE
00363 174* 206 CALL ROCHAR (RDUM,2,-1,5208)
00364 175* NOMIT=,NOMIT+1
00365 176* DECODE (207,RDUM) (OMIT(I),NOMIT,I-1,3)
00373 177* FORMAT(I3A1)
00374 178* GO TO 206
00375 179* 208 CONTINUE
00376 180* MEWR=.TRUE.
00377 181* REVIND N
00400 182* GO TO 203
00400 183* C
00400 184* C BEGIN NAMELIST INPT2
00401 185* 210 CALL PAGI
00402 186* IF (.NOT.,RDYESI) TYPE YES FOR PRINT INPT2 NAMELIST',35') 60 TO 1211
00402 187* C ACCESS THE ORIGINAL NAMELIST FROM PREVIOUS RUN
00404 188* REVIND INAM
00405 189* READ LINAM,INPT2
00410 190* WRITE (6,INPT2)
00413 191* GO TO 1212
00413 192* C RESET ALL PARTS OF NAMELIST
00414 193* 1211 DO 1210 I=1,26
00417 194* MX(I)=0
00420 195* P(I)=0
00421 196* Y(I)=0
00424 197* 1210 V(I)=0
00425 198* TP=.FALSE.
00426 200* HP=.TRUE.
00427 201* TV=.FALSE.
00430 202* UV=.FALSE.
00431 203* SV=.FALSE.
00432 204* RMT=.FALSE.
00433 205* SD=0.0
00434 206* SP=.FALSE.
00435 207* SHOCK=.FALSE.
00436 208* DETN=.FALSE.
00437 209* HMG=.FALSE.
00440 210* PSIA=.TRUE.
00441 211* NSOM=.FALSE.
00442 212* IONS=.FALSE.
00443 213* IDEBUG=0
00444 214* PA=.FALSE.
00445 215* OF=.TRUE.
00446 216* ERATIO=.FALSE.
00447 217* FPCT=.FALSE.
00450 218* GO TO 11211
00450 219* 1212 IF (.NOT.,RDYESI) TYPE YES TO CHANGE NAMELIST',27)
00452 220* X GO TO 203
00454 221* 11211 WRITE (6,211)
00455 222* 211 FORMAT(' BEGIN NAMELIST INPT2 INPUT')
00456 223* 2211 CONTINUE
00456 224* READ (5,INPT2)
00456 225* STORE NAMELIST
00461 226* REVIND INAM
00462 227* WRITE LINAM,INPT2
00465 228* ENDFILE INAM

```

MAIN

```

00464 2280 CALL MOVARS(500.50)
00467 2290 CALL HOLDIT
00470 2300 GO TO 203
00471 2310
00472 2320 215 CONTINUE
00473 2330 FIRST=.FALSE.
00474 2340 CALL PAGIT
00475 2350 CALL GOUT(' ',1)
00476 2360 REMIND INAM
00501 2370 READ (1,INAM,INPT2)
00504 2380 WRITE (6,INPT2)
00505 2390 CALL MOVARS(500.50)
00506 2400 CALL HOLDIT
00507 2410 CALL PAGIT
00510 2420 CALL GOUT(' ',1)
00511 2430 CALL REACT
00514 2440 IF (ICF) 1215,1215,1215 TYPE YES FOR SPECIAL OMITS FOR CAL DATA'.001)
00519 2450 IF (NOT,ADVISE) TYPE YES FOR SPECIAL OMITS FOR CAL DATA'.001)
00516 2460 X GO TO 1215
00521 2470 DO 12 I=1,27
00524 2480 DO 12 J=1,3
00527 2490 12 OMIT(J,OMIT)=1;NOMITS(1,3-3,J)
00530 2500 NOMIT=NOMIT+27
00531 2510 1215 CALCM=.FALSE.
00534 2520 DO 755 I=1,NREAC
00536 2530 IF (NAME(I,6).EQ.12) CALCM=.TRUE.
00540 2540 755 CONTINUE
00542 2550 IF (RATIO) GO TO 213
00545 2560 IF (ICF) 213,1
00550 2570 DO 212 I=1,26
00552 2580 212 MIX(1)=MIX(1)+CF
00555 2590 213 IF (PER-1.0) .214,
00556 2600 NSERT=NSERT+1
00557 2610 ENSERT(1,NSERT)=IC(1)
00560 2620 ENSERT(2,NSERT)=1
00561 2630 ENSERT(3,NSERT)=1
00562 2640 214 CONTINUE
00563 2650 RMOP=0.
00564 2660 VOL=.FALSE.
00565 2670 NT=1
00567 2680 IF (.NOT,TV.AND..NOT.UV.AND..NOT.SV) GO TO 304
00570 2690 VOL=.TRUE.
00573 2700 DO 1304 I=1,26
00575 2710 IF (P(1)) .GT. 0.0) P(1) = 1.0/P(1)
00577 2720 IF (V(1)) .GT. 0.0) P(1) = V(1)
00601 2730 IF (P(1)) .LE. 0.0) GO TO 1305
00603 2740 1304 NP = 1
00604 2750 1305 TP = TV
00605 2760 MP = UV
00606 2770 SP = SV
00607 2780 GO TO 322
00612 2790 304 DO 305 I=1,26
00615 2800 IF (P(1)) .LE. 0.0) GO TO 322
00617 2810 NP = 1
00621 2820 IF (MPHG) P(NP) = P(NP)/760.
00621 2830 IF (PSIA) P(NP) = P(NP)/PATM
00621 2830 IF (NCGM) P(NP) = P(NP)/ATM

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MAIN0000

ORIGINAL PAGE IS
OF POOR QUALITY


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00629 2900 322 DO 307 IT = 1,26
00630 2900 IF (IT11) .LE. 0.01 GO TO 722
00631 2900 IF (CF+1.0) .GT. 1.0 GO TO 722
00632 2900 T11 = T11 - 32.1/1.0 + 273.15
00633 2900 M1 = T11
00634 2900 DO 625 I1 = 1,26
00635 2900 IF (M1I1) .GT. 0.0 GO TO 323
00636 2900 IF (I1I1) .GT. 0.0 GO TO 745
00637 2900 WRITE(OUT,724)
00638 2900 724 FORMAT (//,5X,60M0 IMP2 VALUE GIVEN FOR FA, FPCT, OR OF//)
00639 2900 IF (M1I1) .GT. 0.0 OXFL = M1I1/M1I2
00640 2900 50 TO 333
00641 2900 323 OXFL = MIX(I1I1)
00642 2900 IF (FA) OXFL = 1.0 / MIX(I1I1)
00643 2900 IF (FPCT) OXFL = 100.0 / MIX(I1I1) / MIX(I1I1)
00644 2900 IF (NOT.ERATION) GO TO 333
00645 2900 EORAT = MIX(I1I1)
00646 2900 I1EORAT,EO,1,1 EORAT = 1.000000
00647 2900 OXFL = (1-EORAT+VMIN(2)-VPLS(2))/(VPLS(1)+EORAT+VMIN(1))
00648 2900 333 OXFL(1) = OXFL
00649 2900 625 M0F = 1.5
00650 2900 745 IF (.NOT. IONS .OR. LLMT(L) .EQ. IE) GO TO 746
00651 2900 L = L+1
00652 2900 IF (LLMT(L).NE.1E) MNR = .TRUE.
00653 2900 REMIND = 0
00654 2900 LLMT(L) = IE
00655 2900 POP(L,1) = 0.
00656 2900 POP(L,2) = 0.
00657 2900 GO TO 746
00658 2900 746 IF (LLMT(L).NE.1E) GO TO 746
00659 2900 DO 747 J=1,MS
00660 2900 747 IF (AIL(J).NE. 0.0) IUSE(J) = - 10000
00661 2900 L = L-1
00662 2900 748 IF (MNR) CALL SEARCH
00663 2900 C INITIAL ESTIMATES
00664 2900 SO = SOARRR
00665 2900 ENN = .1
00666 2900 ENNL = -2.3025851
00667 2900 SUMN = ENN
00668 2900 DO 432 J=1,MS
00669 2900 IF (IUSE(J).GT.0) IUSE(J) = -IUSE(J)
00670 2900 IF (IUSE(J).EQ.-10000.AND.IONS) IUSE(J) = 0
00671 2900 EN(J,1) = 0.
00672 2900 EN(J) = 0.
00673 2900 IF (IUSE(J).NE.0) GO TO 432
00674 2900 EN(J,1) = ENN/IONS - NC)
00675 2900 ENLN(J) = ALOG10(EN(J,1))
00676 2900 432 CONTINUE
00677 2900 IOI = L+1
00678 2900 IF (INC.EQ.0.0) INSERT.EQ.0) GO TO 790
00679 2900 DO 302 I=1,MSERT
00680 2900 DO 301 J=1,MS
00681 2900 IF (IUSE(J).EQ.0) GO TO 301
00682 2900 DO 299 I1 = 1,3
00683 2900 299 IF (SUB(I,J,I1).NE. ENLN(I1I1)) GO TO 301
00684 2900 IOI = IOI+1
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MAIN

00764	380*	IUSE(J) = -IUSE(J)	001442
00765	341*	GO TO 302	001444
00766	342*	301 CONTINUE	001452
00770	343*	302 CONTINUE	002452
00772	344*	790 IF (.NOT. TP .AND. .NOT. MP .AND. .NOT. SP) GO TO 791	001452
00774	345*	CALL T4EMP	001456
00775	346*	GO TO 800	001460
00776	347*	791 IF (DET1) CALL DETOM	001462
01000	348*	IF (RT1) CALL ROCKET	001465
01002	349*	IF (SHOCK) CALL SHCK	001471
01004	350*	800 NSERT = 0	001476
01005	351*	CALL MOVARS(800,50)	001476
01006	352*	CALL HOLDIT	001502
01007	353*	GO TO 2	001504
01010	354*	3 CONTINUE	001506
01011	355*	CALL MPSTRM	001506
01012	356*	STOP	001507
01013	357*	END	001513

MAIN0153

END OF COMPILATION: NO DIAGNOSTICS.

ENDG.P MATRIX

MATRIX

STOR,S MATRIX,MATRIX
HSA E3 -10/15/80-13:07:13 (11.)

SUBROUTINE MATRIX ENTRY POINT 001063

STORAGE USED: CODE(1) 001107; DATA(0) 000116; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 POINTS 000335
0004 SPECIES 017104
0005 MISC 001701
0006 DOUBLE 001560
0007 IMOX 000041

EXTERNAL REFERENCES (BLOCK, NAME)

0010 MEMR38

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000102	1246	0001	000103	1276	0001	000126	1406	0001	000215	1546	0001	000244	1616
0001	000472	175L	0001	000677	185L	0001	000953	2176	0001	001011	2304	0001	000567	2446
0001	000406	2476	0001	000623	2576	0001	001026	260L	0001	000757	3036	0001	001023	3176
0001	000276	58L	0001	000346	59L	0001	000372	62L	0001	000376	64L	0001	000511	65L
0001	000405	70L	0001	011052	A	0003	000690	AM	0003	000708	AM1	0003	001135	ANUM
0003	000004	ATOM	0003	R 000514	B0	0003	000545	B0P	0003	000036	CALCH	0004	000000	COEF
0007	L 000001	COMV6	0003	000012	CPR	0003	000706	CPR1	0003	R 000634	CPSUM	0003	000658	DATA
0004	010624	DELM	0003	001560	DEMS	0003	000064	DLVPT	0003	000047	DLVTP	0004	R 004312	EM
0000	R 000013	ENERGY	0004	R 010150	ENLM	0003	001700	ENLSAV	0003	R 000000	ENN	0003	001674	ENML
0005	001677	ENSAYE	0003	001414	ENTH	0003	000636	ERRAT	0003	R 000010	F	0003	001443	FAZ
0005	001527	FOX	0006	0 000000	G	0003	000101	GAMMAS	0007	L 000001	HP	0003	000642	MPP
0003	R 000637	HSUB0	0003	R 000000	HSUM	0004	R 010376	MO	0000	I 000003	I	0007	000030	IC
0007	000000	IDEBUG	0007	I 000015	IMAY	0000	000023	INJPS	0007	000023	IONS	0007	000021	IP
0007	000037	IQSAVE	0007	I 0016	IQ1	0000	I 000001	IQ2	0000	I 000002	IQ3	0007	000005	ISV
0007	000034	IT	0004	I 016266	IUSE	0000	I 000027	J	0007	000026	JL10	0007	000025	JSOL
0005	000463	LLMT	0000	I 000004	K	0000	I 000006	KH	0007	I 000014	KMAT	0007	I 000012	L
0007	000422	NEWR	0007	000040	LSAVE	0007	000006	MOLE	0003	000707	NAME	0007	000024	MC
0007	I 000011	NPT	0007	000035	MF2	0007	000017	MOF	0007	000020	MOHTT	0007	000007	MP
0003	000635	OF	0007	000027	MREAC	0007	I 000013	MS	0000	I 000000	MSPP1	0007	000010	MT
0003	000217	PPP	0003	OC 1644	RH	0003	000116	P	0003	001363	PECVT	0003	000633	PP
0004	R 004064	S	0007	000033	SMOCK	0004	001611	RHOP	0003	001612	RHV	0003	001476	RIEMP
0000	R 000011	SS	0000	R 000005	SS5	0003	000015	SSUM	0004	000251	SOMVEL	0003	000004	SP
0003	R 000003	SD	0003	000150	T	0004	000015	SSUM	0000	R 000012	SUB	0003	R 000001	SUMM
0003	R 000003	TLN	0003	000630	TLOW	0004	000627	TM	0000	000012	TERM1	0003	000632	THIGH
0007	L 000002	TP	0003	R 000002	TY	0003	R 000627	TY	0003	000631	TMID	0003	000320	TOTM
0005	000646	VMIN	0007	L 000012	VOL	0003	000266	TYT	0003	000202	V	0003	000303	VLM
0006	D 001510	X	0003	L 000032	VOL	0005	000650	VPLS	0003	000234	WM	0003	000652	VP

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00101 10 SUBROUTINE MATRIX
00102 20 C
00103 30 COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
00104 40 1.GAMMAS(13),P(26),V(26),V(13),PP(13),UM(13),SONVEL(13),TIT(13)
00105 50 2.VLM(13),TOM(13)
00106 60 C
00107 70 COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENL(150),MO(150)
00108 80 1.DELM(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLM(150)
00109 90 INCLUDE SPECPH
00110 100 COMMON /MISC/ ENM,SUM,TT,SD,ATOM(3,101),LLMT(25),BO(25),
00111 110 1.DOP(25,2),TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EGRAT,
00112 120 2.HSUBD,AN(2),AP(12),RM(2),ENIN(2),VPLS(2),UP(2),
00113 130 3.DAT(25),AM1,CPR1,NAME(25,6),ANUM(25,6),PECNT(25),
00114 140 4.ENTH(25),FAZ(25),RTMP(25),FOX(25),DEMS(25),RMOP,
00115 150 5.RM(25),TLM,ORF(26),ENML,ENSAVE,ENLSAV
00116 160 COMMON /DOUBLE/ G(20,21),X(20)
00117 170 COMMON /IMDX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,MT,MP1,L,MS,
00118 180 1.KMAT,IMAT,IO,MOF,NOMII,IP,HEMR,IONS,NE,JSOI,JL,JO,
00119 190 2.MREAC,IC,JSI,VOL,SMOCH,IT,MFZ,CALCH,IOSAVE,LSAVE
00120 200 C
00121 210 DOUBLE PRECISION 6 X
00122 220 LOGICAL CONVG,MP,SP,TP,VOL
00123 230 IQ2 = IQ1 + 1
00124 240 IQ3 = IQ2 + 1
00125 250 KMAT = IQ3
00126 260 IF(.NOT.CONVG.AND.TP) KMAT = IQ2
00127 270 IMAT = KMAT - 1
00128 280 CLEAR MATRIX STORAGES TO ZERO
00129 290 DO 211 I=1,IMAT
00130 300 DO 211 K=1,KMAT
00131 310 211 G(I,K) = 0.000
00132 320 SSS = 0.
00133 330 MSUM(MPT) = 0.
00134 340 BEGIN SET UP OF ITERATION MATRIX
00135 350 KK = L
00136 360 DO 65 J=1,NS
00137 370 IF(IUSE(J),L,0) GO TO 65
00138 380 IF(IUSE(J),GT,0) GO TO 70
00139 390 F = IMG(J)-SIJ*ENL(J)*THI*EN(J,MPT)
00140 400 SS = MO(J)*EN(J,MPT) - F
00141 410 TERM1 = MO(J)*EN(J,MPT)
00142 420 IF IMAT .EQ. IQ2) TERM1 = F
00143 430 DO 55 I = 1, L
00144 440 CALCULATE THE ELEMENTS RTI,K)
00145 450 IF (ATI,I) .EQ. 0.) GO TO 55
00146 460 DO 15 K=1, L
00147 470 15 G(I,K) = G(I,K) + AIK*J*AI(J)*J*EN(J,MPT)
00148 480 G(I,I) = G(I,I) + AI(I)*I) + AI(J)*EN(J,MPT)
00149 490 G(I,I) = G(I,I) + AI(I)*I) + AI(J)*EN(J,MPT)
00150 500 IF (CONVG .OR. TP) GO TO 55
00151 510 G(I,I) = G(I,I) + AI(I)*I) + AI(J)*EN(J,MPT)
00152 520 IF (SPI) G(I,I) = G(I,I) + AI(I)*I) + AI(J)*EN(J,MPT)
00153 530 SS CONTINUE
00154 540 IF IMAT .EQ. IQ2) GO TO 64
00155 550 IF (CONVG .OR. MP) GO TO 59
00156 560
00157 570
00158 580
00159 590
00160 600
00161 610
00162 620
00163 630
00164 640
00165 650
00166 660
00167 670
00168 680
00169 690
00170 700
00171 710
00172 720
00173 730
00174 740
00175 750
00176 760
00177 770
00178 780
00179 790
00180 800
00181 810
00182 820
00183 830
00184 840
00185 850
00186 860
00187 870
00188 880
00189 890
00190 900
00191 910
00192 920
00193 930
00194 940
00195 950
00196 960
00197 970
00198 980
00199 990
00200 1000

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MATRIX

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00202 500 G1122,1011 = G1102,1011 + SS      000323
00203 510 G1102,1021 = G1102,1021 + H01J10SS      000326
00204 520 G1102,1031 = G1102,1031 + S1J1 - ENLM(J1-TM)*F      000330
00205 530      0 TO 62      000340
00206 600 G1102,1021 = G1102,1021 + H01J1020*EN(J,MPT1)      000346
00207 610      IF (CONV6) 60 TO 64      000362
00208 620 G1102,1031 = G1102,1031 + H01J1031*F      000364
00209 630 G1102,1031 = G1102,1031 + F      000372
00210 640 G1102,1021 = G1102,1021 + TERM1      000376
00211 650      60 TO 65      000403
00212 660 C CONDENSED SPECIES      000403
00213 700 AR = AR + 1      000408
00214 800 DO 75 I = 1,L      000407
00215 810 G11,MM1 = A11,J1      000453
00216 820 G11,MM1 = G11,MM1 - A11,J1*EN(J,MPT1)      000454
00217 830 G11,MM1 = H01J1      000462
00218 840 G11,MM1 = H01J1 - S1J1      000465
00219 850 HSUM(MPT1) = HSUM(MPT1) + H01J1*EN(J,MPT1)      000471
00220 860      IF (NOT-S1) 50 TO 65      000477
00221 870 SSS = SSS + S1J1*EN(J,MPT1)      000501
00222 880 G1102,MM1 = S1J1      000505
00223 890 C CONTINUE      000520
00224 900 SSS = SSS + G1102,1011      000529
00225 910 HSUM(MPT1) = HSUM(MPT1) + G1102,1021      000537
00226 920 G1102,1011 = SSS - ENM      000537
00227 930 C REFLECT SYMMETRIC PORTIONS OF THE MATRIX      000543
00228 940 K = 101      000542
00229 950      IF (MP-OR-CONV6) K = 102      000606
00230 960 DO 102 I = 1,K      000606
00231 970 DO 102 J = 1,K      000606
00232 980 G1J,11 = G1J,J1      000606
00233 990 C COMPLETE THE RIGHT HAND SIDE      000606
00234 1000      IF (CONV6) 60 TO 175      000612
00235 1010 DO 105 I = 1,L      000623
00236 1020 X11 = 0111-G11,1011      000623
00237 1030 G1J,MM1 = G1J,MM1 + X11      000625
00238 1040 G1102,MM1 = G1102,MM1 + ENM-SUMM      000630
00239 1050 C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN      000630
00240 1060      IF (MM1-EO-102) 60 TO 105      000636
00241 1070      IF (MP1) ENM = 50*ENM-SUMM - SSS      000641
00242 1080      IF (MP1) ENM = HSUM(MPT1)      000654
00243 1090 G1102,1021 = G1102,1021 + ENM      000665
00244 1100      IF (NOT-VOL-OR-CONV6) RETURN      000672
00245 1110 C CONSTANT VOLUME MATRIX      000677
00246 1120 K = 101 - 1      000704
00247 1130      IF (MM1-EO-102) 60 TO 210      000707
00248 1140 DO 220 I = 1,K      000721
00249 1150 G1102,11 = G1102,11 + G1102,11      000757
00250 1160 G11,1011 = G11,1021 - G11,1011      000761
00251 1170      220 G11,1021 = G11,1031      000764
00252 1180 G1102,1011 = G1102,1021 - G1102,1011      000767
00253 1190 G1102,1021 = G1102,1031 - G1102,1011      000774
00254 1200      IF (MP) G1102,1021 = G1102,1021 + ENM      001001
00255 1210 GO TO 240      001007
00256 1220 DO 240 I = 1,K      001011

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MATRIX

00321	1120	240	611,1011 = 611,1021	001023
00323	1130	250	KMAT = IMAT	001026
00324	1140		IMAT = IMAT-1	001027
00325	1150		RETURN	001031
00326	1160		END	001106

MATX0070

END OF COMPILATION: NO DIAGNOSTICS.

AM06.P OUT1

OUT1

370P.5 OUT1 OUT1
MSA E3 -10/15/80-13:07:10 (15,)

SUBROUTINE OUT1
ENTRY POINT 002156
OUT2
OUT3
OUT4
ENTRY POINT 002167

STORAGE USER: CONCL1, 002172; DATA10 000655; BLANK COMMENT2) 000000

COMMON BLOCKS:

0003 COMSTS 000004
0004 HOLCOM 000010
0005 POINTS 000335
0006 SPECES 017106
0007 MISC 001701
0010 INDR 000041
0011 PLRF 002166
0012 CUPY 000073
0013 CC 000003
0014 CRUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0015 VAFMT
0016 MOVARS
0017 HOLCIT
0020 PAGIT
0021 MUDUS
0022 M1018
0023 M1028
0024 M1036
0025 SORT
0026 MEMRS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	0003	17	0001	000034	10L	0001	001440	10146	0001	001443	10206	0001	001470	10346
0001	001477	10426	0001	001510	10456	0001	001520	10506	0001	001544	10646	0001	001573	10726
0001	001621	11076	0001	001627	11156	0001	001643	11246	0001	001673	11356	0001	001752	11536
0001	001760	11616	0001	002030	11766	0001	002042	12056	0001	002054	12146	0001	002066	12236
0001	002100	12326	0001	002112	12416	0001	003044	130L	0001	000025	1346	0001	001120	140L
0001	000043	1646	0001	001144	170L	0001	003152	175L	0001	001221	177L	0001	001257	179L
0001	001261	180L	0000	000377	2F	0000	000333	20F	0001	000112	2006	0001	001334	200L
0001	000371	210L	0001	001373	211L	0000	000353	22F	0000	000310	240F	0001	000213	2476
0001	000335	2416	0001	000276	2776	0000	000404	280F	0000	000422	290F	0001	000036	30L
0000	000450	300F	0000	000452	310F	0001	000320	3106	0000	000416	320F	0001	000334	3216
0001	000362	3326	0000	000412	340F	0001	000404	3416	0001	000420	3506	0001	000447	3446
0001	000471	3746	0001	000501	4036	0001	000522	4146	0001	000544	4256	0001	000560	4326
0001	000604	4446	0001	000615	45L	0001	000623	4556	0001	000647	4716	0000	000471	490F
0000	000612	492F	0001	000217	50L	0001	001451	500L	0001	000670	5126	0000	000477	504F

OUT1

0001	001533	504L	0001	001536	510L	0001	000711	5136	0001	00104	514L	0001	000225	52													
0000	000504	520E	0001	000717	5206	0000	000511	524F	0000	000734	5276	0000	000517	537F													
0001	000753	537E	0000	000525	542F	0000	000532	544F	0001	000763	5456	0000	000540	546F													
0000	000546	546F	0000	000554	550F	0000	000562	552F	0001	001007	5556	0001	001075	6106													
0001	001100	6136	0001	001106	6206	0001	001131	6316	0001	001149	6366	0001	000163	6416													
0001	001157	6506	0001	001216	6616	0001	001247	6736	0001	001275	7156	0001	001307	7206													
0001	001331	7276	0001	000342	7416	0001	001362	7416	0000	000405	80F	0004	011052	A													
0011	000150	AFAT	0007	000640	AM	0007	000705	AM	0007	R	001135	AMUM	0011	000133	APP												
0003	P	000000	AFAT	000004	ATOM	0007	000514	BO	0007	000545	BOF	0010	000036	CALCH													
0014	P	000000	CF	000103	CMV	0006	000000	COEF	0000	R	000047	CNF	0010	000001	COMVG												
0005	R	000032	CPR	000706	CPM	0007	000634	CPSUM	0007	000654	DATA	0006	010624	DELM													
0013	P	000002	DEMAND	0001560	DEMS	0005	R	000044	DLVPT	0005	R	000027	DLVPT	0000	R	000236	DOL										
0000	R	000147	EE	0004312	EM	0004	000000	END	0004	010150	ENLM	0007	001700	ENLSAV	0007	000188	EOL										
0007	000000	ENM	0007	001676	ENML	0007	001677	ENSAVF	0007	R	001414	ENTM	0011	L	000005	FB	0012	R	000005	FB							
0007	R	000436	EQRAT	000002	FA	0012	R	000003	FAP	0007	R	001445	F2	0012	R	000015	FC	0012	R	000015	FC						
0012	000004	FC	0012	000007	FCP	0012	R	000012	FCS7	0012	R	000014	FCV	0012	R	000000	F2R	0012	R	000000	F2R						
0012	000017	FGE	0012	000020	F6V	0012	R	000021	FM	0000	R	000036	FMM	0012	R	000023	F1	0012	R	000023	F1						
0012	R	000025	FIV	000027	FM	0012	R	000031	FMT	0012	R	000050	FM	0012	R	000052	FOUP	0012	R	000052	FOUP						
0007	I	001527	FOX	000053	FP	0000	R	000046	FPC	0000	R	000032	FPP	0012	R	000034	FS	0012	R	000034	FS						
0000	R	000040	FSS	0012	R	000056	F5V	0012	R	000057	FT	0012	R	000041	FTM	0000	R	000034	FTM	0000	R	000034	FTM				
0012	R	000043	FV	0012	R	000065	FVEL	0000	R	000001	FVLM	0012	R	000001	F13	0012	R	000000	F2R	0012	R	000000	F2R				
0005	R	000101	GAMMAS	0004	R	000011	G4S	0003	R	000001	GMET	0010	R	000003	GRAPH	0000	R	000003	HEAD	0000	R	000003	HEAD				
0000	P	000321	HWD	000152	H4VS	0004	R	000001	H4V	0010	R	000001	H4V	0007	R	000042	MPP	0007	R	000042	MPP	0007	R	000042	MPP		
0007	000437	HSUMD	0005	R	000000	HSUM	0006	R	010376	HO	0000	I	00002	I	0000	I	000030	IC	0000	I	000030	IC	0000	I	000030	IC	
0018	000000	IDEBUG	0000	I	000261	IOE	0004	R	000002	IE	0000	I	000050	IFLAG	0000	I	000104	IJ	0000	I	000104	IJ	0000	I	000104	IJ	
0010	000037	IMAT	0000	I	000253	IOX	0000	R	000424	INJPS	0010	R	000023	IOXS	0010	R	000021	IP	0010	R	000021	IP	0010	R	000021	IP	
0004	I	016244	IUSE	000016	IOI	0004	R	000045	J	0010	R	000045	J	0010	R	000045	J	0010	R	000045	J	0010	R	000045	J		
0000	R	000025	J5OL	000033	I2	0000	R	000043	K	0010	R	000043	K	0010	R	000043	K	0010	R	000043	K	0010	R	000043	K		
0000	R	000046	LMYD	000031	J51	0000	R	000051	L4VS	0007	R	000043	LLM?	0010	R	000043	LLM?	0010	R	000043	LLM?	0010	R	000043	LLM?		
0000	I	000306	L3	000037	L4	0000	R	000037	L4	0004	R	000005	MOL	0010	R	000005	MOL	0010	R	000005	MOL	0010	R	000005	MOL		
0007	I	000070	NAME	000024	MC	0010	R	000024	MC	0000	I	000044	MD	0010	R	000044	MD	0010	R	000044	MD	0010	R	000044	MD		
0010	I	000012	MLM	000017	MOF	0010	R	000017	MOF	0010	R	000020	MOKIT	0010	R	000020	MOKIT	0010	R	000020	MOKIT	0010	R	000020	MOKIT		
0010	I	000027	MPAC	0010	I	000033	MS	0000	I	000000	MSPP1	0010	R	000000	MSPP1	0010	R	000000	MSPP1	0010	R	000000	MSPP1	0010	R	000000	MSPP1
0012	P	000067	OF	0004	I	000006	OX	0007	R	001444	ORF	0005	R	000016	P	0005	R	000016	P	0005	R	000016	P	0005	R	000016	P
0011	000000	PCP	0007	R	001363	PECWT	0014	R	000003	PER	0007	R	000033	PP	0005	R	000033	PP	0005	R	000033	PP	0005	R	000033	PP	
0003	R	000003	REAR	0003	R	000004	REAR	0007	R	000644	RM	0007	R	001611	RMOP	0007	R	001611	RMOP	0007	R	001611	RMOP	0007	R	001611	RMOP
0007	R	001474	RTMP	0003	R	000005	RYR	0004	R	000044	S	0010	R	000033	SMOCK	0004	R	000033	SMOCK	0004	R	000033	SMOCK	0004	R	000033	SMOCK
0005	R	000251	SOMVEL	0010	R	000004	SP	0011	R	000047	SPIM	0005	R	000018	SSUM	0005	R	000018	SSUM	0005	R	000018	SSUM	0005	R	000018	SSUM
0011	000101	SUBAR	0004	R	000303	SUM	0007	R	000001	SUMM	0011	R	000016	SUPAR	0007	R	000016	SUPAR	0007	R	000016	SUPAR	0007	R	000016	SUPAR	
0005	000150	T	0004	R	016514	TEMP	0007	R	000032	THIGH	0007	R	000032	THIGH	0012	R	000032	THIGH	0012	R	000032	THIGH	0012	R	000032	THIGH	
0007	000630	TLOW	0007	R	000427	TM	0007	R	000631	TMID	0005	R	000320	TOTM	0010	R	000320	TOTM	0010	R	000320	TOTM	0010	R	000320	TOTM	
0007	000002	TY	0005	R	000266	TYT	0012	R	000071	TWO	0012	R	000071	TWO	0005	R	000071	TWO	0005	R	000071	TWO	0005	R	000071	TWO	
0005	R	000033	VLM	0007	R	000646	VHIM	0011	R	000032	VMOG	0011	R	000032	VMOG	0010	R	000032	VOL	0010	R	000032	VOL	0010	R	000032	VOL
0014	R	000002	WCR	0005	R	000244	WM	0007	R	000652	WP	0007	R	000652	WP	0000	R	000652	XDP	0000	R	000652	XDP	0000	R	000652	XDP
0000	R	000135	YDPS	0000	R	000020	YH	0000	R	000025	YX	0000	R	000025	YX	0006	R	010376	Z	0006	R	010376	Z	0006	R	010376	Z
0012	000072	ZEROF																									

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OUT1P0001
/COMSTS/
/MOLCOM/

COMMON /COMSTS/ ATMM,CMET,PATH,PAR,RR,RRR,RRR
COMMON /MOLCOM/ FND,GAS,IC,IZ,LANK,MOL,OX,ZERO
COMMON /OUT1P/MSUM(I3),SSUM(I3),CP(I3),DLVPT(I3),DLVPT(I3)

00101
00101
00101
00101
00101

OUT1

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00105 1 GAMMAS(13),P(26),T(26),V(13),PPP(13),MM(13),SONVEL(13),TTT(13) 000000
00115 2 VLM(13),TOTM(13) 000000
00105 C COMMON/SPICES/COEF(2,7,150),S(150),EN(150),EN(150),EN(150),H(150) 000000
00105 C 1 DELM(150),A(150),SUB(150,3),IUSE(150),TEMPI(50,2),SLN(150) 000000
00106 INCLUDE SPICPR 000000
00112 COMMON /MISC/ ENMSUMN,TT,SO,ATOM(13,101),ELMT(25),BO(25), 000000
00112 1 BQ(12,5,2),TM,TLOW,THIGH,PP,CP,SUM,OF,ECORAT, 000000
00112 HSUBD,AM(2),MPP(2),RM(2),VM(2),VPLS(2),MP(2), 000000
00112 3 DATA(25),AM,CPRI,NAME(25,6),ANUM(25,6),PECUT(25), 000000
00112 4 ENTH(25),FAZI(25),ATEMP(25),FOX(25),OENS(25),RHOP, 000000
00112 5 RM(25),TLN,OXF(26),ENML,ENSAVE,ENLSAV 000000
00113 COMMON /INDEX/ IDEBUG,CONVG,IP,HP,SP,ISV,MOLES,PMPT,NLM,MS, 000000
00113 1 RMAT,IMAT,IOI,NOF,NOIMIT,IP,MEWR,IONS,MC,USOL,LIO, 000000
00113 2 NREAC,IC,JSI,VOL,SHOCK,IT,NFZ,CALCH,IOSAVE,LSAVE 000000
00114 COMMON /PERF/ PCPI(26),MOC(13),SPIN(13),VACI(13),SUBAR(13), 000000
00114 1 SUPAR(13),APP(13),AEAT(13),EOL 000000
00115 COMMON /OUP1/ FOX,F13,FA,API(2),FB,FC,FCPI(3),FCI(2),FCV,F(2), 000000
00115 1 FSE,FEV,FH(2),EII(2),FIN(2),EN(2),MT(13),EN(2),FOUR, 000000
00115 2 FP,FS(2),FSV,FT(2),FTN(2),FV(2),FVEL(2),ONE,THREE, 000000
00115 3 TWO,ZERO 000000
00115 C COMMON /CCC/GRAPH,JOUT,DEMAND 000000
00116 COMMON /CFUEL/CF,MHV,VCR,PER 000000
00117 C DIMENSION FVLM(2),HEAD(9),MW(2,2),VM(5),YX(5),Z(10,3) 000000
00120 DIMENSION EPP(2),FTRI(2),FHM(2),FSS(2) 000000
00120 1 DATA 'PPI1',I=1,21,'PRESS ','PSIA ' 000000
00120 2 DATA 'FTRI',I=1,21,'TEMP O ','EG F ' 000000
00120 3 DATA 'FHM',I=1,21,'ENTH B ','TU/LB ' 000000
00120 4 DATA 'FSS',I=1,21,'S.OIV ','ILB-R1' 000000
00120 5 EQUIVALENCE IZ,MQI 000000
00120 6 INTEGER FOX,OX 000000
00120 7 LOGICAL EOL,MOLES,VOL 000000
00120 C HEAD = (1XA6,2X51A2,F8-5,3X), 5X,F7-5,F13-3,4X,A1,F10-2,F9-4) 000000
00120 1 DATA HEAD/6H(1XA6),6H2X51A2,6H,F8-5,6H,3X), 5,6H,F7-5,6H,F13-3, 000000
00120 2 6H,4X,A1,6H,F10-2,6H,F9-4),YM/6H2X1A2,6H2X2(A2,6H2X3(A2, 000000
00120 3 6H2X(A2,6H2X5(A2),YX/6H3X),57,6H3X),44,6H3X),31,6H3X),18, 000000
00120 4 3 6H3X), 5,MW/24HWT FRACTION MOLES /,FVLM/12HVOLUME CC/G / 000000
00120 C K = 1 000000
00120 IF (MOLES) K = 2 000001
00120 WRITE(JOUT,240) MW(1,K),MW(2,K) 000005
00120 240 FORMAT (7X,2A6,34M ENTHALPY STATE TEMP DENSITY/10X, 000025
00120 1 16CHEMICAL FORMULA,65X,THCAL/MOL,10X,6HODEG. K,3X,5H6/CM3) 000025
00120 DO 60 K = 1,NREAC 000025
00120 IF (FOX(K).NE. OX) GO TO 10 000025
00120 MD = 6HODONT 000030
00120 GO TO 30 000032
00120 10 MD = 6HFUEL 000034
00120 DO 40 J=1,5 000036
00120 30 IF(IANUM(K,J)).LE. O. .OR. NAMEIN(J).EQ. LANK) GO TO 45 000043
00120 J=6 000045
00120 45 J=J-1 000065
00120 HEAD(2) = YN(J) 000073

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OUT 1

DATE 101500

PAGE

5

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00400 1180 70 CONTINUE
00401 1190 IF (IFLAG.EQ.0) WRITE (JOUT,1) (V(I),J=1,NPT)
00402 1200 1 FORMAT (1X,14H DENSITY G/CC,1P13E9.3)
00403 1210 IF (IFLAG.EQ.1) WRITE (JOUT,2) (V(I),J=1,NPT)
00404 1220 2 FORMAT (1X,14H DENSITY L/F003,1P13E9.3)
00405 1230 WRITE(JOUT,80)
00406 1240 80 FORMAT (1X,1)
00407 1250 C MOLECULAR WEIGHT
00408 1260 WRITE(JOUT,FMT) FM,FB,WM(J), J = 1,NPT)
00409 1270 C (DLV/DLPIT
00410 1280 IF (EQL) WRITE(JOUT,FMT) FT,FB,(DLVPT(J), J = 1,NPT)
00411 1290 C (DLV/DLIR
00412 1300 IF (EQL) WRITE(JOUT,FMT) FV,FB,(DLVPT(J), J = 1,NPT)
00413 1310 C HEAT CAPACITY
00414 1320 DO 85 I=1,NPT
00415 1330 85 V(I) = RBAR*CPH(I)
00416 1340 WRITE(JOUT,FMT) FCP,(V(I), J = 1,NPT)
00417 1350 C GAMMA(S)
00418 1360 WRITE(JOUT,FMT) FG,FB,(GAMMA(S(J), J = 1,NPT)
00419 1370 FMT(4) = TWO
00420 1380 DO 95 I = 1,NPT
00421 1390 95 SONVEL(I) = SORT(RBAR*GAMMA(S(I),TTT,I,WM(I))
00422 1400 WRITE(JOUT,FMT) FSI,FVEL,(SONVEL(I), J = 1,NPT)
00423 1410 CALL MOVAPS(500,50)
00424 1420 CALL MOLDIT
00425 1430 CALL PAGIT
00426 1440 RETURN
00427 1450 C
00428 1460 ENTRY OUT1
00429 1470 IF (CF=1.0) .130,
00430 1480 COF=CF/CF
00431 1490 WRITE (JOUT,22) COF,NCR,PER
00432 1500 130 WRITE (JOUT,80)
00433 1510 ND = 0
00434 1520 C MOLE FRACTIONS EQUILIBRIUM OR FROZEN
00435 1530 WRITE(JOUT,280)
00436 1540 280 FORMAT (19H MOLE FRACTIONS/)
00437 1550 IF (.NOT. EQL) GO TO 175
00438 1560 EQUILIBRIUM MOLE FRACTIONS
00439 1570 DO 170 M=1,NS
00440 1580 DO 140 I=1,NPT
00441 1590 140 V(I) = EMR,I/(TOTM(I)
00442 1600 DO 150 I=1,NPT
00443 1610 150 IF (V(I)) .GE. 5.0E-7) GO TO 160
00444 1620 ND = 1
00445 1630 GO TO 170
00446 1640 160 WRITE(JOUT,340) (SUBIN(J), J = 1,3),FB,(V(I), I = 1,NPT)
00447 1650 340 FORMAT (1H,34A,A2,1P13E9.3)
00448 1660 170 CONTINUE
00449 1670 C OUTPUT COMPLETE GO EXIT
00450 1680 GO TO 211
00451 1690 175 FROZEN MOLE FRACTIONS
00452 1700 J = 0
00453 1710 DO 179 M = 1,NS
00454 1720 V(J+1) = FM,K,1/(TOTM(I)
00455 1730
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01013 2290 DO 502 I=1,NPT
01016 2300 SUM=0.
01017 2310 DO 500 J=1,NS
01022 2320 IF (IUSE(J),NE.0) GO TO 500
01023 2330 SUM=SUM+EM(J,I)/TOTN(I)
01027 2340 500 CONTINUE
01027 2350 CHW(I)=SUM(I)*SUM
01030 2360 502 CONTINUE
01032 2370 WRITE (JOUT,504) (CHW(I),I=1,NPT)
01040 2380 504 FORMAT (X,MIXTURE MW,AX,13F9.5)
01041 2390 C LOCATE DRY ELEMENTS
01041 2400 DO 510 I=1,6
01044 2410 DO 508 J=1,NS
01047 2420 DO 506 K=1,3
01052 2430 IF (I06(I,K),NE.15UG(J,K)) GO TO 508
01054 2440 506 CONTINUE
01056 2450 IMX(I)=J
01057 2460 GO TO 510
01060 2470 508 CONTINUE
01062 2480 IMX(I)=0
01063 2490 510 CONTINUE
01065 2500 DO 516 I=1,NPT
01070 2510 SUM=0.
01071 2520 DO 514 J=1,6
01074 2530 IJ=IMX(J)
01075 2540 IF (IJ.EQ.0) GO TO 514
01077 2550 SUM=SUM+EM(IJ,I)
01100 2560 514 CONTINUE
01102 2570 XDP(I)=SUM/TOTN(I)
01103 2580 516 CONTINUE
01105 2590 WRITE (JOUT,520) (XDP(I),I=1,NPT)
01113 2600 520 FORMAT (X,MF OF CDG,5X,13F9.5)
01114 2610 DO 522 I=1,NPT
01117 2620 YDPS(I)=(305.2*XDP(I)/CHW(I))*(1./CF)*(1.+OF)
01120 2630 522 CONTINUE
01122 2640 WRITE (JOUT,524) (YDPS(I),I=1,NPT)
01130 2650 524 FORMAT (X,Y SAT SCF/LB,2X,13F9.5)
01131 2660 L1=IMX(1)
01132 2670 L3=IMX(3)
01133 2680 L4=IMX(4)
01134 2690 DO 530 I=1,NPT
01137 2700 SUM=0.
01140 2710 IF (L4.NE.0) SUM=SUM+319.2*EM(L4,I)/TOTN(I)
01142 2720 IF (L1.NE.0) SUM=SUM+316.0*EM(L1,I)/TOTN(I)
01144 2730 IF (L3.NE.0) SUM=SUM+994.0*EM(L3,I)/TOTN(I)
01146 2740 HWS(I)=SUM/XDP(I)
01147 2750 530 CONTINUE
01151 2760 WRITE (JOUT,532) (HWS(I),I=1,NPT)
01157 2770 532 FORMAT (X,MHV SAT B/SCF,1X,13F9.2)
01160 2780 DO 538 I=1,NPT
01163 2790 EE(I)=HWS(I)*YDPS(I)/MHV
01164 2800 YDP(I)=379.5*YDPS(I)/385.2
01165 2810 MHVD(I)=(385.2/379.5)*HWS(I)
01166 2820 IF (L4.NE.0) LHSV(I)=HWS(I)-(1059.9*18./385.2)*EM(L4,I)/TOTN(I)
01166 2830 X /XDP(I)
01170 2840 LHSV(I)=(HWS(I)*345.2/379.5
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01171 285* DOL(1)=10000.*((1.25*HHVV/10000.*OF/CF)/(HHVS(I)*VDPS(I)))
01172 286* S30 CONTINUE
01174 287* WRITE (JOUT,542) ((E(I),I=1,NPT)
01202 288* S42 FORMAT (1X,'EFFICIENCY',4X,13F9.5)
01203 289* WRITE (JOUT,544) (YD(I),I=1,NPT)
01211 290* S44 FORMAT (1X,'Y DRY SEE/LB',2X,13F9.5)
01212 291* WRITE (JOUT,546) (HHV(I),I=1,NPT)
01220 292* S46 FORMAT (1X,'HHV DRY B/SCF',1X,13F9.2)
01221 293* WRITE (JOUT,548) (LHVS(I),I=1,NPT)
01227 294* S48 FORMAT (1X,'LHV SAT B/SCF',1X,13F9.2)
01230 295* WRITE (JOUT,550) (LHVD(I),I=1,NPT)
01236 296* S50 FORMAT (1X,'LHV DRY B/SCF',1X,13F9.2)
01237 297* S52 WRITE (JOUT,552) (DOL(I),I=1,NPT)
01245 298* S52 FORMAT (1X,'S PER MBTU',3X,13F9.2)
01246 299* S60 CONTINUE
01247 300* RETURN
01250 301* ENO

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OUTP0137

END OF COMPILATION: 1 DIAGNOSTICS.

ENDG,P

PROK

PROK

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APDP,LMF PROK PROK
F0P12R1 R72-16,10/15/80 13:07:27 (0,0) RI
PE0001 SPECPR PROC
0002 COMMON/SPECES/COEF(2,7,150),S(150),EMI(150,13),EMLN(150),MO(150)
0003 1,DELN(150),A(15,150),SUB(15,0,3),TUSE(150),TEMP(50,2),SLN(150)
0004 DATA NSPP1/151/
0005 END

END PDP ERRORS : NONE

ENDG,P REACT

REACT

3FOR,S REACT,REACT
MSA 23 -10/15/80-13:07:28 (31.)

SUBROUTINE R_{ACT} ENTRY P₀INT 001077

STORAGE USED: CODE(1) 001111; DATA(0) 000367; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 HOLCON 000010
0004 MISC 001701
0005 IMOX 000041
0006 CCC 000003
0007 CFUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0010 OUT
0011 RMCOOS
0012 MOVARS
0013 HOLBYT
0014 PAGIT
0015 NREWS
0016 MRBUS
0017 NIOZS
0020 NIOIS
0021 MYDUS
0022 MERR3S

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STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000327	101L	0001	000003	1326	0001	000013	1436	0001	000072	18L	0001	000074	20L
0001	000463	200L	0001	000521	204L	0001	000106	206L	0001	000557	210L	0001	000315	212F
0001	000566	214L	0001	000736	218L	0001	000740	220L	0001	001002	222L	0001	001005	224L
0001	001022	226L	0001	001042	229L	0001	001056	230L	0001	000146	2326	0001	000233	2476
0001	000243	275G	0000	000301	30F	0001	000256	304G	0001	000300	3176	0001	000377	3426
0001	000226	37L	0001	000512	4008	0001	000534	4148	0001	000554	4306	0001	000617	4476
0001	000270	45L	0001	000275	46L	0001	000662	4606	0001	000712	4736	0001	000311	50L
0001	000766	510G	0001	000771	513G	0001	001012	531G	0001	001033	5436	0001	001046	5526
0001	000042	6L	0004	000640	AM	0004	000705	AM1	0004	000707	ANAME	0004	001135	ANUM
0004	000004	ATOM	0004	000514	BO	0004	000545	BOF	0005	000336	CALCH	0007	000000	CF
0005	000001	CONV8	0004	000706	CPRI	0004	000634	CPSUM	0004	000654	DATA	0006	000002	DEMAND
0004	001560	DENS	0003	000000	END	0004	001700	ENLSAV	0004	000000	ENM	0004	001676	ENML
0004	001677	ENSAVE	0004	001814	ENTH	0004	000636	FORAT	0004	001445	FAT	0004	001527	FOX
0003	000001	GAS	0006	000000	GRAPH	0004	000001	HVV	0005	000003	HP	0004	000642	MPP
0004	000637	MSUBO	0000	000262	I	0005	000030	IC	0005	000000	IDEBUG	0003	000002	IE
0005	000015	IMAT	0000	000344	INJPS	0000	000271	IO	0005	000023	IONS	0000	000235	IOUT
0005	000021	IP	0005	000037	IOSAVE	0005	000016	IO1	0005	000005	ISV	0005	000034	IT
0003	000003	IZERO	0000	000266	J	0000	000275	JJ	0005	000026	JL10	0006	000001	JOUT
0005	000025	J50L	0005	000031	J51	0000	000265	K	0005	000014	KMAT	0005	000012	L
0003	000004	LANK	0000	000145	LINE1	0000	000172	LINE2	0000	000215	LINE3	0004	000463	LLMT
0000	000032	LIMITS	0005	000040	LSAVE	0003	000005	MOL	0000	000272	MOLE	0005	000006	MOLES


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0000 I 000270 N
0005 L 000022 NEWR
0005 000017 NOF
0005 000013 NS
0003 I 000006 OX
0004 000033 PP
0004 R 001976 RTEMP
0004 000003 SO
0004 000431 TM
0005 000032 VOL
0004 I 000707 NAME
0000 I 000267 MFUEL
0005 I 000020 NM
0005 001644 OXF
0004 R 000044 RH
0000 P 000063 SGP
0004 000032 THIGH
0005 000002 TP
0004 R 000050 VPLS
0000 I 000273 MAST
0005 000035 NFZ
0005 000007 NP
0000 I 000263 N3
0000 R 000276 PCY
0000 001611 RMHP
0005 000033 SHOCK
0005 001643 TLH
0004 000002 TT
0007 R 000002 VCR
0005 000024 MC
0000 I 000000 MLS
0005 000000 MPT
0000 I 000264 M8
0004 R 001363 PECUT
0004 R 000274 RM
0004 000004 SP
0004 000030 TLOW
0004 R 000001 V
0004 R 000266 VM
0005 I 000267 ZERO

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00101 SUBROUTINE REACT
00101 C
00103 COMMON /MOLCON/ EMO,GAS,IE,IZERO,LAMB,MOL,OX,ZERO
00104 COMMON /MISCZ/ EMIN,SUMM,IT,SG,ATON(13,103),LLMT(26),Q(138),
00104 BOP(25,2),TM,TLOW,IMIO,THIGH,PP,CP,SUM,OF,EGRAT,
00104 MSUBO,AM(2),MPP(2),RM(2),VMIN(2),VPLS(2),UPI(2),
00104 DATA(25),AM1,CPM1,NAME(25,6),ANUM(25,6),PECUT(25),
00104 ENTH(25),FAZ(25),RTMP(25),FOX(25),DENS(25),RHOP,
00104 RMV(25),TLM,OXF(26),EMML,EMSAVE,CM,SAV
00105 COMMON /IMOX/ IOEUBG,CONIG,IP,MP,SP,ISX,MOLES,MP,ML,MPI,L,MS,
00105 KMAT,IMAT,IQI,NOF,NOMIT,IP,NEWR,TONS,MC,JSOL,JL10,
00105 MREAC,IC,JSI,VOL,SHOCK,IT,MFZ,CALCM,IQSAVE,LSAVE
00105 C
00105 COMMON /CC/ GRAPH,JOUT,DEMAND
00105 C
00105 COMMON /CFUEL/CF,MHVV,VCR,PER
00105 DATA NLS/O/
00105 DIMENSION ANAME(25,6),V(25),LLMTS(25),SBOPI(25,2)
00105 EQUIVALENCE (NAME,ANAME)
00105 INTEGER FOX,OX,ZERO
00105 LOGICAL MOLES,NEWR
00105 DIMENSION LINE(21),LINE2(19),LINE3(16)
00105 DIMENSION IOUT(21)
00105 DATA ILINE(1),I=1,21)/' INDEX',40,'
00105 X 'REACTA','MT(1)',30,' R',
00105 X 'EL MT',' MOL','E ENT','HALPY','
00105 X ' PHA','SE TE','MP,M ' ' FUEL',' DENS','ITY ' /
00105 DATA ILINE2(1),I=1,19)/100,'
00105 X ' N','O MOLE','S ' ' INT',
00105 X ' EMERG','Y ' '20,' ' OXID ' /
00105 DATA ILINE3(1),I=1,16)/80,'
00105 X ' ' ' ' ' IND','ICATES',' ENTHA','LPY TO',' BE CA',
00105 X 'LCULAT','ED ' /
00105 C
00105 DATA M3/8/,N8/12/
00105 C
00105 DO 8 K = 1,2
00105 MPIN=0
00105 MPP(M)=0
00105 RMIN=0
00105 VPLS(M)=0

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00190 430 VMIN(M)=0.
00191 000 AMIN(M)=0.
00192 450 DO 8 J=1,25
00193 460 LLMT(J)=0
00194 470 DO 1 J=1, 0.0
00195 480 MFUEL = 0
00196 490 N=1
00197 500 C WRITE REACTANT HEADER
00198 510 CALL GOUTLINE1,126,
00199 520 CALL GOUTLINE2,110,
00200 530 L=1
00201 540 IO=M3
00202 550 C READ REACTANTS
00203 560 REWIND IO
00204 570 6 READ (IO) MREAC,CF
00205 580 10 IF (10.EQ.MR) GO TO 20
00206 590 IF (CF,1.0) ,10.
00207 600 REWIND IC
00208 610 READ (M3) MREAC,CF,MH,MY,MCR,PER
00209 620 10 IF (MREAC.EQ.0) GO TO 200
00210 630 20 CONTINUE
00211 640 READ (M3) (NAME(M,I),ANUMIN(I),I=1,5),PECT(M),MOLE,EXT(M),
00212 650 X NAME(M,6),ANUMIN(6),FAZIN,
00213 660 X RIENP(M),LE,OX(N),DENS(M)
00214 670 MAST=1M
00215 680 IF (NAME(M,6).EQ.2M00) MAST=1M
00216 690 ENCODE (30,10UT) M,NAME(M,J),ANUMIN(J),J=1,5),PECT(M),MOLE,
00217 700 X ENTH(M),MAST,FAZIN),RIENP(M),FOXIN),DENS(M)
00218 710 CALL GOUT(10UT,126)
00219 720 30 FORMAT (1X,12X,51A2,F0.9,2X1,F10.6,2X,A3,F13.4,A1,F12.3,
00220 730 X 3X,A1,F12.5,1X)
00221 740 IFIL.EQ.0160 TO 20
00222 750 IF (MOLE.EQ.0) MOLES = .TRUE.
00223 760 IF (OXICANT, K = 1: IF FUEL, K = 2.
00224 770 IF (FOXIN).EQ.0) FOXIN=OX
00225 780 IF (PECT(M).LE.0.0) PECT(M) = 1.0
00226 790 K = 1
00227 800 IF (FOXIN).EQ.0) GO TO 37
00228 810 K = 2
00229 820 MFUEL = MFUEL+1
00230 830 37 DO 10 J=1,25
00231 840 38 DATA(J) = 0.0
00232 850 RM=0.
00233 860 DO 100 JJ=1,6
00234 870 IF (ANUMIN(JJ).LE.0.0) GO TO 101
00235 880 IF (NAME(M,JJ).EQ.0) NAME(M,JJ) = OX
00236 890 DO 41 J=1,15
00237 900 I = J
00238 910 IF (LLMT(J).EQ.0) GO TO 45
00239 920 IF (NAME(M,JJ).EQ.0) LLMT(JJ) GO TO 46
00240 930 L = I
00241 940 LLMT(JJ)=NAME(M,JJ)
00242 950 DO 48 I = 1,101
00243 960 48 IF (ATOM(I,1).EQ.0) ANAME(M,JJ) GO TO 50
00244 970 L=0
00245 980 GO TO 20

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00326 990 50 RM = RM + ANUMIN,JJ)*ATOM(2,I)
00327 1000 V(J) = ATOM(2,I)
00330 1010 100 DATA(J) = ANUMIN,JJ)
00332 1020 101 PCMT=PCMT+RM
00333 1030 IF(MOLES) PCMT=PCMT*RM
00335 1040 MPIN=MPIN + PCMT
00336 1050 IF (NAMEIN,6) NE,1ZER0) MPIN(K)=MPIN(K)+[MINMIN)*PCMT/RM
00339 1060 AMIN=AM,MI,PCMT/RM
00341 1070 DO 110 J=1,L
00344 1080 110 BOP(J,K) = DATA(J)*PCMT/RM + BOP(J,K)
00346 1090 IF (DENSE,MI) .GT. 0.0) RM(K) = RM(K) + PCMT/DENSE(MI)
00350 1100 RM(K) = RM
00351 1110 N = N+1
00352 1120 IF (IN,EO,26) GO TO 200
00359 1130 IF (IO,EO,N3,AND,N-1,EO,NREAC) GO TO 200
00364 1140 IF (IO,EO,N3,AND,N-1,EO,N3) N3 EAC) GO TO 200
00366 1150 GO TO 20
00368 1160 200 NMIN=N-1
00369 1170 IF (IO,EO,N3) GO TO 200
00370 1180 IO=N3
00372 1190 REVIND IO
00374 1200 READ (10) NREAC,CF,MWV,UCR,PER
00375 1210 IF (NREAC,EO,0) GO TO 200
00377 1220 DO 202 J=1,N
00402 1230 READ (10) NDUIMY
00405 1240 202 CONTINUE
00407 1250 GO TO 6
00410 1260 204 NREAC=NMI
00411 1270 IF (FUEL,GT,0) GO TO 210
00413 1280 C 100 PERCENT OXIDANT, CALL REACTANTS FUEL
00415 1290 DO 205 N=1,NREAC
00416 1300 205 FOR(N) = LANK
00420 1310 RM(2) = RM(1)
00421 1320 RM(1) = 0.
00422 1330 MP(2) = MP(1)
00423 1340 MP(1) = 0.
00424 1350 MP(2) = MP(1)
00425 1360 AM(2) = AM(1)
00426 1370 AM(1) = 0.
00427 1380 DO 208 J=1,L
00432 1390 208 BOP(J,2) = BOP(J,1)
00434 1400 210 IF (L,NC,0) GO TO 214
00436 1410 WRITE (10),212)
00440 1420 212 FORMAT ('0',ERROR IN REACTANT DATA')
00441 1430 214 CALL GOUTLINE(3,96)
00442 1440 CALL GOUTLINE(3,96)
00443 1450 CALL MOVABS(500,50)
00444 1460 CALL MOLOTY
00445 1470 CALL PAGIT
00446 1480 DO 220 N=1,2
00451 1490 IF (MPIN) .LE. 0.0) GO TO 220
00453 1500 MPIN=MPIN/MPIN)
00454 1510 AMIN = MPIN/AMIN)
00455 1520 IF (RMIN) .GT. 0.0) RMIN = MPIN/RMIN)
00457 1530 DO 215 J=1,L
00462 1540 BOP(J,1)=BOP(J,1)/MPIN)

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00063 1550 IF (V(J), LT 0, VMIN(K) = VMIN(K) + BOP(J,K) * V(J) 000664
00065 1560 IF (V(J), .GT. 0.0) VPLS(K) = VPLS(K) + BOP(J,K) * V(J) 000673
00070 1570 IF (MOLES) GO TO 220 000705
00072 1580 DO 218 N=1, NREAC 000712
00075 1590 IF (FOX(N).EQ.OX.AND.K.EQ.2).OR.(FOX(N).NE.OX.AND.K.CO.1) GO TO 218 000712
00077 1600 PECH(N) = PECH(N) / MP(K) 000732
00080 1610 218 CONTINUE 000742
00082 1620 220 CONTINUE 000742
00084 1630 NEWR=.TRUE. 000742
00086 1640 C ARE ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEWR=.FALSE. 4/23/70 000742
00088 1650 IF (L.NE.MLS.OR.NOMIT.NE.O) GO TO 226 000744
00090 1660 DO 224 I=1,MLS 000756
00092 1670 DO 222 J=1,L 000771
00094 1680 IF (LLMT(J).NE.LLMTS(I)) GO TO 222 000771
00096 1690 SROP(I,1) = BOP(J,1) 000774
00098 1700 SROP(I,2) = BOP(J,2) 000776
00100 1710 GO TO 224 001000
00102 1720 222 CONTINUE 001003
00104 1730 GO TO 226 001003
00106 1740 224 CONTINUE 001006
00108 1750 NEWR=.FALSE. 001006
00110 1760 DO 225 I=1,L 001012
00112 1770 LLMT(I) = LLMTS(I) 001012
00114 1780 SROP(I,1) = SROP(I,1) 001013
00116 1790 SROP(I,2) = SROP(I,2) 001015
00118 1800 GO TO 229 001020
00120 1810 226 MLS = L 001022
00122 1820 REWIND 9 001023
00124 1830 DO 228 I=1,L 001026
00126 1840 SROP(I,1) = BOP(I,1) 001033
00128 1850 SROP(I,2) = BOP(I,2) 001034
00130 1860 LLMTS(I) = LLMT(I) 001036
00132 1870 228 LLMTS(I) = LLMT(I) 001042
00134 1880 229 DO 230 N=1,NREAC 001046
00136 1890 IF (DENS(N).GT.0.0) GO TO 230 001050
00138 1900 PH(2) = 0. 001051
00140 1910 RH(1) = 0. 001051
00142 1920 RETURN 001052
00144 1930 230 CONTINUE 001057
00146 1940 RETURN 001057
00148 1950 END 001110

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END OF COMPILATION: NO DIAGNOSTICS.

AMOG,P RKTOUT

ARON. S. ARNOLD, AR YOU?

ENTRY POINT 000532

STORAGE USED: COOL(1), DODS4: PAYAID) D00122: BLANK COMMON(2) 000000

Common Blocks:

0003	COMETS	000006
0004	POINTS	000035
0005	SPECIES	017106
0006	INDEX	000041
0007	PIEF	000166
0010	DUPT	000073
0011	CCC	000003
0012	CFJZ	000001

GENERAL REFERENCES (BLOCK NAME)

0013	0013	MYVANS
0014	0014	OUT1
0015	0015	VAFMY
0016	0016	OUT2
0017	0017	GAMFF
0020	0020	OUT3
0021	0021	OUT4
0022	0022	WFOUS
0023	0023	NI02S
0024	0024	NI01S
0025	0025	SORT
0026	0026	NI01S
0027	0027	WFOUS

STORAGE ASSIGNMENT	BLOCK	TYPE	RELATIVE LOCATION	NAME
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	4	4	4	4
5	5	5	5	5
6	6	6	6	6
7	7	7	7	7
8	8	8	8	8
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12	12	12	12	12
13	13	13	13	13
14	14	14	14	14
15	15	15	15	15
16	16	16	16	16
17	17	17	17	17
18	18	18	18	18
19	19	19	19	19
20	20	20	20	20
21	21	21	21	21
22	22	22	22	22
23	23	23	23	23
24	24	24	24	24
25	25	25	25	25
26	26	26	26	26
27	27	27	27	27
28	28	28	28	28
29	29	29	29	29
30	30	30	30	30
31	31	31	31	31
32	32	32	32	32
33	33	33	33	33
34	34	34	34	34
35	35	35	35	35
36	36	36	36	36
37	37	37	37	37
38	38	38	38	38
39	39	39	39	39
40	40	40	40	40
41	41	41	41	41
42	42	42	42	42
43	43	43	43	43
44	44	44	44	44
45	45	45	45	45
46	46	46	46	46
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87	87	87	87	

0001	000063	146C	0000	000046	150F	0001	000074	1546	0001	000121	1706	000150	2006
0001	000202	200L	0000	000075	208F	0001	000022	220L	0001	000235	2226	0001	000243
0001	000316	254G	0001	000040	2646	0001	000350	2746	0001	000366	3056	0001	000511
0001	000044	321G	0001	000047	3266	0001	000445	3376	0001	000466	3506	0001	000505
0000	000006	37F	0000	000027	38F	0000	000056	40F	0001	000520	404L	0000	000047
0005	011052	A	0007	000150	4F4Y	0007	R	000133	APP	0003	R	000000	4M
0004	000036	CALCH	0012	000000	CF	0005	000000	COLF	0006	000001	COMYS	0000	000032
0000	000005	C57R	0005	010424	DELM	0011	000002	DEMAND	0004	000049	DLUPT	0000	000047
0005	004312	EP	0005	010150	EMLM	0007	L	000165	EOL	0010	R	000002	FAP
0010	000005	F4	0010	000006	FC	0010	000007	FCL	0010	R	000012	FCSY	FCA
0010	000015	FC	0010	R	000017	F6E	0010	R	000020	FAY	0010	R	000023
0010	000025	F1V	0010	000027	F4	0010	R	000031	FMT	0010	R	000030	FM
0010	000053	F1V	0010	000054	FS	0010	000056	F5V	0010	000057	FT	0010	000061
0010	000061	FV	0010	R	000065	FVEL	0010	R	000001	FJ3	0010	R	000101
0001	000001	G1V	0011	000000	SP4PH	0006	000003	MP	0004	R	000000	MSUM	NO
0000	000004	I	0004	000013	IC	0004	000000	10CPUS	0005	000015	1MAT	0007	000105
0000	000004	I	0004	000013	IC	0004	000000	10CPUS	0005	000015	1MAT	0007	000105

[illegible]

10	00101	SUBROUTINE MKTOUT (IGAM)	000000
20	00101		000000
30	00101		000000
40	00101		000000
50	00101		000000
60	00104	COMMON /CONST/ ATW,GMET,PATH,RRAB,ROR,RVR	000000
70	00104	COMMON /POINT/MSUM(13),ASSUM(13),CPR(13),OLVTP(13),OLVPT(13)	000000
80	00104	1 GAMMA(13),PI(26),T(26),V(13),PP(13),MM(13),SONVEL(13),VT(13)	000000
90	00104	2 VLM(13),JOTM(13)	000000
100	00104	COMMON /SPEC/ COEF(12),T(13),S(13),EM(150),MLM(150),MO(150)	000000
110	00105	1 DELW(150),A(15,150),SUB(150,3),IUSE(150),TEMP(150,2),SLM(150)	000000
120	00111	INCLUDE SPECPR	000000
130	00111	COMMON /IMOX/ IDEBUG,CONVE,TP,NOP,SP,ISV,MOLES,MP,MT,NPT,NLM,MS,	000000
140	00111	1 HMA,IMAT,OL,NOR,NOMIT,IP,MEVR,IONS,MC,JOL,JLLO,	000000
150	00112	2 NPEAC,ICJ(3),VOL,SHOCK,IT,NFZ,CALCM,IOSAVE,LSARC,	000000
160	00112	COMMON /PERF/ PC(124),MOC(13),SPIM(13),VACI(13),SUMAR(13),	000000
170	00112	1 SUPAR(13),APP(13),ACAT(13),COL	000000
180	00113	COMMON /OUP/ F2X,F13,FA,FAP(2),FB,FC,FCP(3),FCST(2),FCV,FC(2),	000000
190	00113	1 FBE,F6V,F(12),F(12),F(12),F(12),FM(2),FM(15),FM(2),FOUR,	000000
200	00113	2 F(12),F(12),F(12),F(12),F(12),F(12),F(12),F(12),F(12),F(12),	000000
210	00113	3 TWO,ZERO	000000
220	00114	COMMON /CCC/ GRAPH,JOUT,DEMAND	000000
230	00114		000000
240	00115	COMMON /CFUEL/CF	000000
250	00116	LOGICAL EOL	000000
260	00117	CALL MOVARS(500,501)	000000
270	00120	IF (COL) WRITE(JOUT,37)	000003
280	00123	37 FORMATION(1)/24X,BNTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM	000012
290	00123	10M COMPOSITION DURING EXPANSION	000012
300	00124	IF (NOT COL) WRITE(JOUT,38)	000012
310	00127	38 FORMATION(1),24X,BNTHEORETICAL ROCKET PERFORMANCE ASSUMING PROZEN	000023
320	00127	10M COMPOSITION DURING EXPANSION	000023
330	00130	IF (VT(11).EQ.74111) WRITE(JOUT,337)	000023
340	00133	337 FORMAT (52X,20HAT AM ASSIGNED TEMPERATURE	000034
350	00134	TEM = PATHMOPPI1)	000034
360	00135	AM = ATWOPPP(1)	000037
370	00136	WRITE(JOUT,40) TEM,AM	000037
380	00142	40 FORMAT (5H FC =,F10.3,7H PSIA =,1PE13.6,7H M/MOO2)	000051
390	00143	CALL OUT1	000051
400	00143	AM = NPT - 2	000051

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00145 410 DO 20 I = 1,K 000056
00150 420 V(I) = HEXIT 000063
00152 430 WRITE(JOUT,150) (V(I), I = 1,K) 000065
00160 440 FORMAT (1H0,16X,16HCHAMBER THROAT,11(SX,AN)) 000077
00162 450 C PRESSURE RATIOS 000077
00164 460 FMT(13) = ONE 000077
00166 470 CALL VARFMT (APP,NPT) 000101
00168 480 WRITE(JOUT,FMT) FC,F8,FB,(APP(I), I = 1,NPT), 000105
00170 490 CALL OUT2 000124
00172 500 IF INPT .LT. 21 GO TO 312 000126
00174 510 DO 202 K=2,NPT 000136
00176 520 SPIM(K) = SORT(2,0,ORR+(HSUM(I,1 - HSUN(K)),1)/GMET 000150
00178 530 C AU (A/W) IN UNITS OF SEC/ATM 000150
00180 540 AV = BR+TTT(K)/(PP(K)*UM,K)*SPIM(K)*GMET**2) 000161
00182 550 IF (K.NE.216) TO 200 000171
00184 560 CSTR = GMET*AV*PP(1) 000174
00186 570 AEAT(2) = 1. 000177
00188 580 200 VACI(K)=SPIM(K)*PP(K)*AV 000202
00190 590 IF (SONVEL(K) .GT. 0.0) VMOC(K) = GMET*SPIM(K)/SONVEL(K) 000205
00192 600 202 V(K) = GMET*SPIM(K) 000214
00194 610 V(1) = 0.0 000221
00196 620 WRITE(JOUT,FMT) FGV,FVEL,(V(I), I = 1,NPT) 000222
00198 630 C MACH NUMBER 000222
00200 640 FMT(4) = FOUR 000240
00202 650 VMOC(1) = 0. 000242
00204 660 IF (GAMMA(2) .LE. 0.0) VMOC(2) = 0.0 000243
00206 670 WRITE(JOUT,FMT) FM,FB,(VMOC(I), I = 1,NPT) 000247
00208 680 WRITE(JOUT,208) 000266
00210 690 208 FORMAT (1H ) 000273
00212 700 C AREA RATIO 000273
00214 710 CALL VARFMT (AEAT,NPT) 000273
00216 720 FMT(3) = F9X 000301
00218 730 WRITE(JOUT,FMT) FA,FB,FB,(AEAT(I), I = 2,NPT) 000303
00220 740 C CSTAR 000303
00222 750 FMT(4) = F13 000321
00224 760 FMT(5) = TWO 000323
00226 770 WRITE(JOUT,FMT) FCST,FB,(CSTR, I = 2,NPT) 000325
00228 780 C CF - THRUST COEFFICIENT 000325
00230 790 FMT(5) = FOUR 000343
00232 800 DO 212 I=2,NPT 000350
00234 810 V(I) = GMET*SPIM(I)/CSTR 000354
00236 820 WRITE(JOUT,FMT) FC,FB,FB,(V(I), I = 2,NPT) 000371
00238 830 IF (IGAM .EQ. 0) GO TO 220 000371
00240 840 C EFFECTIVE GAMMA 000371
00242 850 CALL GAMEFF IV,GAMMA,APP,NPT,HO) 000373
00244 860 WRITE(JOUT,FMT) FGI,FGI,FGI,FGI, I = 2,NPT) 000402
00246 870 C VACUUM THRUST COEFFICIENT 000402
00248 880 DO 230 I = 2,NPT 000427
00250 890 V(I) = GMET*VACI(I)/CSTR 000433
00252 900 C VACUUM IMPULSE 000450
00254 910 FMT(5) = THREE 000452
00256 920 WRITE(JOUT,FMT) FIV,FB,(VACI(I), I = 2,NPT) 000452
00258 930 C SPECIFIC IMPULSE 000471
00260 940 WRITE(JOUT,FMT) FI,FB,(SPIM(I), I = 2,NPT) 000471
00262 950 C FROZEN MOLE FRACTION OUTPUT MOVED TO SURROUTINE OUT3 000471
00264 960 000471

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RTOUT

00364	97*	312 CALL OUT3	000511
00365	98*	IF (CF*1.0) *000.	000512
00370	99*	CALL OUT4	000515
00371	100*	*00 CONTINUE	000520
00372	101*	RETURN	000520
00373	102*	END	000540

END OF COMPILATION: NO DIAGNOSTICS.

ANDG.P ROCKET

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AFOR,S ROCKET,ROCKET
HSA E3 -10/15/80-13:07:36 (10.1)

SUBROUTINE ROCKET ENTRY POINT 001310

STORAGE USED: CODE(1) 001317: DATA(0) 000231: BLANK COMMON(2) 000000

COMMON BLOCKS:

0001 CONSTS 000006
0004 POINTS 000335
0005 MISC 001701
0006 INOX 000041
0007 PERF 000146
0010 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0011 MEMOF
0012 FROZEN
0013 EOLBRM
0014 RMTOUT
0015 SAVE
0016 MDOUS
0017 NIO2S
0020 NMNLS
0021 NMNLS
0022 XPRR
0023 ALO6
0024 EXP
0025 XPOR
0026 SORT
0027 MERRIS

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000013	1256	0001	000162	1332L	0001	000035	1446	0001	000054	1566	0000	000104	1811F
0001	000302	191L	0001	00020	192L	0000	000101	194F	0001	000261	195L	0001	000126	2036
0000	000065	302F	0001	00026	303L	0001	000045	306L	0001	000103	321L	0001	000122	322L
0001	000153	331L	0001	000160	332L	0001	000175	333L	0001	000213	334L	0001	000610	799L
0001	000536	600L	0001	000763	802L	0001	000640	805L	0001	000703	809L	0001	000653	810L
0001	001007	820L	0000	000125	821F	0001	001015	830L	0001	001043	834L	0001	001053	835L
0001	001055	859L	0001	001061	860L	0000	000137	862F	0000	000166	865F	0001	001121	870L
0001	001135	880L	0001	00057	899L	0001	000377	900L	0000	000073	923F	0001	000416	925L
0001	001171	990L	0001	001232	997L	0001	001264	999L	0007	000150	ATAT	0000	000037	ACATL
0005	000640	AM	0005	000705	AM1	0005	001135	ANUM	0007	000133	APP	0000	000035	APPL
0000	000033	ARAT10	0000	000005	AREA	0000	000001	ASQ	0003	000000	ATMN	0005	000004	ATOM
0000	000030	AVT	0005	000514	BO	0005	000545	BOP	0006	000036	CALCH	0006	000001	CONV6
0004	000072	CPH	0000	000023	CPHF	0005	000706	CPR1	0005	000634	CPSUM	0005	000654	DATA
0010	000002	DEMAND	0005	001560	DEMG	0000	000026	DH	0000	000032	DLMP	0000	000040	DLNPE
0000	000027	DLT	0004	000044	DLVPT	0004	000047	DLVTF	0000	000034	ELM	0005	001700	ENLSAV
0005	000000	ENH	0005	001676	ENML	0005	001677	ENSAVE	0005	001414	ENTH	0007	000165	EQL

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0005 000636 EORAT      0005 001495 FAZ      0005 001527 FOX      0000 L 000006 FROZ      0004 R 000101 GAMMAS
0003 000001 GHET      0000 000000 GRAPH      0006 L 000003 HP      0005 000642 MPP      0005 000637 MSUBO
0004 R 000000 HSUM      0000 I 000012 I      0006 000030 IC      0000 I 000000 ICASE      0006 I 000000 IDEBUG
0000 I 000011 IGAM      0000 000015 IMAT      0000 000215 IMJPS      0000 I 000016 IOF      0006 000023 IOMS
0000 I 000021 IP      0000 I 000022 IPP      0006 000037 IOSAVE      0006 000016 IOI      0000 I 000020 ISUP
0000 I 000021 ISUP      0006 I 000005 ISV      0006 I 000034 IT      0000 I 000037 ITNUM      0000 I 000025 ITROT
0006 000026 JLIO      0010 I 000001 JOUT      0006 I 000025 JSOL      0006 000031 JSI      0006 000014 KMAT
0005 000463 LLMT      0006 000040 LSAVE      0006 000006 MOLES      0005 000024 MC      0006 000024 NC
0006 000022 NEUR      0006 I 000035 FZ      0006 000012 MLM      0006 I 000017 MOF      0006 000020 MOMIT
0000 I 000007 NP      0000 I 000013 MPP      0006 I 000011 MPT      0006 000027 MREAC      0006 000013 MS
0000 I 000014 MSUR      0000 I 000015 MSUP      0006 I 000010 MT      0005 R 001644 OXF      0005 R 001644 OXF
0004 R 000116 P      0003 R 000002 PATH      0007 R 000000 PCP      0000 R 000031 PCPLT      0005 001363 PCNT
0005 R 000633 PP      0004 R 000217 PPP      0003 000003 RBR      0003 R 000004 RRR      0005 000644 RH
0003 001811 RHOP      0000 000041 RNTIMP      0005 001612 RMV      0003 001876 RTEMP      0003 000005 RVR
0000 L 000007 SEQL      0006 000033 SHOCK      0004 000251 SONVEL      0006 L 000004 SP      0007 000047 SPIH
0000 R 000015 SSUM      0007 R 000101 SUBAR      0005 000001 SUMM      0007 R 000116 SUPAR      0005 R 000003 SO
0004 R 000150 T      0000 L 000010 TMI      0005 000632 THIGH      0005 001643 TLM      0005 000630 TLOW
0005 000527 TM      0000 R 000024 TMELT      0005 000633 TMID      0000 R 000036 TOL      0004 000320 TOTM
0006 L 000002 TP      0005 R 000002 TT      0004 R 000266 TTT      0000 D 000003 USO      0004 000202 V
0007 000064 VACI      0004 000333 VLM      0005 000646 VMIM      0007 000032 VMOC      0006 000032 VOL
0005 000650 VPLS      0004 R 000234 VM      0005 000652 VP

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00101 SUBROUTINE ROCKET
00101 1* C
00101 2* C
00101 3* C
00101 4* C
00101 5* C
00101 6* C
00101 7* C
00101 8* C
00101 9* C
00101 10* C
00101 11* C
00101 12* C
00101 13* C
00101 14* C
00101 15* C
00101 16* C
00101 17* C
00101 18* C
00101 19* C
00101 20* C
00101 21* C
00101 22* C
00101 23* C
00101 24* C
00101 25* C
00101 26* C
00101 27* C
00101 28* C
00101 29* C
00101 30* C
00101 31* C

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ROCKET PERFORMANCE

COMMON /CONSTS/ ATMM,GMEI,PAIM,RBAR,RBR,RVR
COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),DLVTP(13),OLVPT(13)
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),MM(13),SONVEL(13),TTT(13)
2 ,VLM(13),TOTM(13)
COMMON /MISC/ ENMSUMM,TI,SO,ATON(3,101),LLMT(25),BO(25),
BOPI(25,2),TM,TLOW,THIGH,PP,CP,SUM,OF,EORAT,
MSUBO,AM(2),MPP(2),RH(2),VJM(2),VPLS(2),IMP(2),
DATA(25),AMI,CPRI,NAME(25,6),ANUM(25,6),PECM(25),
ENTH(25),FAZI(25),RTEMP(25),FOX(25),DEMS(25),RHOP,
RMW(25),TLM,OXF(26),ENML,ENMSAVE,ENLSAV
COMMON /INDX/ IDEBUG,COMB6,TP,NP,SP,ISV,MOLES,NP,MT,NPT,MLM,MS,
KMA,IMAT,IOI,NOF,MOMIT,IP,MEWR,IOMS,NC,JSOL,JLTO,
MREAC,IC,JSI,VOL,SHOCK,IT,MFZ,CALCM,IOSAVE,LSAVE
COMMON /PERF/ PCPI(26),VMOC(13),SPIN(13),VACI(13),SUBAR(13),
SUPAR(13),APP(13),ACAT(13),EQL
1
COMMON /CCC/ GRAPH,JOUT,DEMAND
COMMON /CASE/O/
DOUBLE PRECISION ASO,USO
LOGICAL AREA,EQL,FROZ,HP,SEQL,SP,TMI,TP
NAMELIST /RNTIMP/ EQL,FROZ,IGAM,PCP,SUBAR,SUPAR
NFX = 1
APP(1) = 1.
IF (ICASE .GT. 0) GO TO 303

ROCKET

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00122 320 ICASE = 1
00123 330 IGAM = 0
00124 340 DO 300 I=1,26
00127 350 PCP(I) = 0.
00130 360 SUBAR(I) = 0.0
00132 370 EQL = .TRUE.
00133 380 FRZ = .FALSE.
00134 390 WRITE (6,302)
00136 400 302 FORMAT (' BEGIN NAMELIST RTIMP INPUT')
00137 410 303 READ (5,RTIMP)
00142 420 NPP = 0
00143 430 DO 305 I = 1,26
00146 440 IF (PCP(I) .LE. 0.0) GO TO 306
00150 450 305 MPP = I
00152 460 306 MPP = MPP*2
00153 470 NSUB = 8
00154 480 NSUP = 0
00155 490 DO 320 I=1,13
00160 500 IF (SUBAR(I) .GT. 0.0) NSUB = NSUB + 1
00162 510 IF (SUBAR(I) .GT. 0.0) NSUP = NSUP + 1
00165 520 WRITE(JOUT,RTIMP)
00170 530 SEQL = EQL
00171 540 IOF = 0
00172 550 II = 3800.
00173 560 C LOOP FOR EACH O/F
00174 570 321 IT = 1
00175 580 IOF = IOF + 1
00176 590 OF = OF(IOF)
00177 600 CALL NEWOF
00178 610 IF (IT) .LE. 0.0) GO TO 322
00179 620 IT = IT + 1
00201 630 C LOOP FOR CHAMBER PRESSURES
00202 640 322 DO 998 IP = 1,MP
00205 650 ITNUM = 0
00206 660 AREA = 0
00207 670 IF (IT) .LE. 0.0) MP = .TRUE.
00211 680 IF (IT) .GT. 0.0) TP = .TRUE.
00213 690 SP = .FALSE.
00214 700 EQL = .TRUE.
00215 710 ISUB = 1
00216 720 ISUP = 1
00217 730 PP = P(IIP)
00220 740 IPP = 1
00221 750 C LOOP FOR PRESSURE RATIOS
00222 760 331 IF (EQL) GO TO 332
00223 770 CALL FROZEM
00224 780 GO TO 1332
00225 790 332 CALL EOLBPM
00226 800 C TT = 0 IF NO CONVERGENCE
00227 810 1332 IF (IT .GT. 0.0) GO TO 333
00228 820 IF (IMPT .LT. 2) RETURN
00229 830 GO TO 900
00230 840 333 IF (IPP .GT. 1) GO TO 195
00231 850 C COMRUSSION CHAMBER
00232 860 EQL = SEQL
00233 870 TP = .FALSE.
00236

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ROCK0060
ROCK0062

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ROCKET

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00474 2000 001116
00475 2010 001121
00476 2020 001123
00500 2030 001125
00502 2040 001132
00503 2050 001139
00504 2060 001140
00506 2070 001193
00510 2080 001154
00512 2090 001163
00513 2100 001167
00514 2110 001171
00516 2120 001176
00520 2130 001203
00522 2140 001206
00523 2150 001210
00524 2160 001285
00525 2170 001217
00526 2180 001221
00527 2190 001222
00530 2200 001224
00531 2210 001225
00532 2220 001230
00533 2230 001232
00534 2240 001233
00536 2250 001240
00540 2260 001244
00542 2270 001250
00544 2280 001254
00545 2290 001260
00546 2300 001262
00547 2310 001264
00551 2320 001272
00552 2330 001316

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870 NPT = 2
 IF (.NOT. EQL) GO TO 880
 IF (ISV.EQ.1) ISV = -1
 CALL SAVE
 880 IPP = IPP + 1
 IF (NPT.EQ.2) GO TO 331
 IF (.NOT. AREA) APPINPT = PCP(IPP-2)
 IF (AREA) APPINPT = EXP(AMPL)
 PP = P(IPP)/APPINPT
 GO TO 331
 990 IF (IOBUG.LI.0) IOBUG = IOBUG + 1
 IF (MSUB.LI.0) MSUB = -MSUB
 IF (.NOT. FROZ.OR. .NOT. EQL) GO TO 997
 CPR(1) = CPRF
 GAMMA(1) = CPRF/(CPRF-1./WM(1))
 TT = TTT(1)
 IPP = 1
 NPT = 1
 CALL SAVE
 EQL = .FALSE.
 ENM = 1./WM(1)
 GO TO 334
 997 NPT = 1
 WRITE(10UT,065)
 IF (ISEQL) CALL SAVE
 998 TT = TTT(1)
 IF (ITT.GE.MT) GO TO 999
 IT = IT + 1
 TT = TTT(1)
 GO TO 322
 999 IF (IOF.GE. .NOF) RETURN
 GO TO 321
 ENO

END OF COMPILATION: NO DIAGNOSTICS.

ENDG,P PREAD

RREAD

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FOR S RREAD, RREAD
MSA 'E3 -10/15/80-13:07:40 (26.)

SUBROUTINE RREAD ENTRY POINT 001330

STORAGE USED: CODE(1) 001345; DATA(0) 001373; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CFUEL 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0004 ROYES
0005 PAGIT
0006 CHRSLZ
0007 GOUT
0010 MNCODS
0011 RDATAI
0012 RDATAF
0013 DMVRIE
0014 ROCHAR
0015 MRBUS
0016 MRBUS
0017 MIOZS
0020 NIOIS
0021 NERRZB
0022 NVRUS
0023 MVEFS
0024 NERR3B

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000014	10L	0001	00277	100L	0001	000375	106L	0001	000437	110L	0001	000517	120L
0001	000551	130L	0001	000605	140L	0001	000623	150L	0001	000644	160L	0001	000662	170L
0001	000011	176G	0001	000703	200L	0001	000045	2026	0001	000116	2326	0001	000134	2426
0001	000747	300L	0001	001032	310L	0001	000326	3226	0001	001062	330L	0001	001110	340L
0001	000366	346G	0001	001127	350L	0001	001144	360L	0001	000454	3656	0001	001163	370L
0001	000501	376G	0001	001201	400L	0001	001216	408L	0001	001305	420L	0001	000716	4506
0001	000717	4536	0001	000070	50L	0001	000770	501G	0001	001015	5126	0001	001210	5656
0001	001221	602G	0001	001235	6066	0001	001276	6356	0001	000177	70L	0000	001276	802F
0001	000240	90L	0001	000274	95L	0000	R 000226	ANUM	0003	R 000000	CF	0000	R 000702	DENS
0000	P 000536	FNTH	0000	R 001125	EXMP1A	0000	R 001140	EXMP1B	0000	R 001150	EXMP2	0000	R 001156	EXMP2B
0000	R 001163	EXMP3	0000	R 001170	EXMP3B	0000	R 001177	EXMP4	0000	R 001203	EXMP5	0000	R 001207	EXMP6
0000	R 001214	EXMP7	0000	R 000567	FA7	0000	R 000651	FOX	0000	I 001252	I	0000	I 001257	ICMG
0000	001347	INJMS	0000	I 001250	IO	0000	I 001255	IOPT	0000	I 001023	IOUT	0000	I 001220	IREACT
0000	I 001253	J	0000	I 001236	LINEO	0000	I 000733	LINE1	0000	I 000760	LINE2	0000	I 001003	LINE3
0000	I 001050	MOOIFY	0000	I 001065	MOOEM	0000	I 000505	MOLE	0000	I 001256	M	0000	I 000000	NAME
0000	I 001254	MAST	0000	I 001260	MDUMMY	0000	I 001251	MREAC	0000	I 001246	M3	0000	I 000000	NAME
0000	000454	PECVY	0000	P 001224	RDUM	0000	L 000000	RDYFS	0000	P 000620	RTEMP			

READ

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00162 560 C READ IN PRESENT CASE 000006
00162 570 C CONTINUE 000006
00164 580 10 IF (IO.EQ.N3) REWIND 10 000014
00165 590 READ (IO) NREAC,CF 000014
00167 600 IF NREAC.LT.11 GO TO 50 000021
00173 610 DO 25 I=1,NREAC 000027
00175 620 READ (IO) (NAME(I,J),J=1,5),PECT(I),MOLE(I), 000033
00200 630 X ENTH(I),NAME(I,6),ANUM(I,6),FAZ(I),RTEMP(I),FOR(I),DENS(I) 000041
00200 640 CONTINUE 000070
00220 650 C 000070
00220 660 C DISPLAY PRESENT SET OF REACTANTS (ADD IF NONE EXIST) 000070
00222 680 C CONTINUE 000070
00223 690 CALL PAGIT 000071
00224 700 CALL CHRSTZ(9) 000074
00225 710 IF (NREAC.LT.11) GO TO 70 000100
00227 720 CALL GOUTLINE1,125) 000104
00230 730 CALL GOUTLINE2,119) 000116
00231 740 DO 60 I=1,NREAC 000116
00234 750 NAST=1M 000116
00235 760 IF (NAME(I,6).EQ.2M00) NAST=1M0 000120
00237 770 ENCODE(102,1OUT,1,NAME(I,J),ANUM(I,J),J=1,5),PECT(I),MOLE(I), 000125
00237 780 X ENTH(I),NAST,FAZ(I),RTEMP(I),FOR(I),DENS(I) 000125
00257 790 CALL GOUT(1OUT,125) 000151
00260 800 C CONTINUE 000162
00262 810 CALL GOUT(' ',1) 000162
00263 820 CALL GOUTLINE3,92) 000166
00264 830 CALL GOUT(' ',1) 000172
00265 840 CONTINUE 000177
00266 850 CALL GOUT(MODIFY,75) 000177
00267 860 IOPT=0 000202
00270 870 CALL RDATA(1,IOPT,870) 000203
00271 880 IF (IOPT.LT.0 .OR. IOPT.GT.3) GO TO 70 000210
00273 890 IF (IOPT.EQ.0) GO TO 90 000225
00275 900 GO TO (90,90,300),IOPT 000227
00275 910 C 000227
00275 920 C SELECT REACTANT NUMBER 000227
00276 930 CONTINUE 000240
00277 940 N=1 000241
00300 950 IF (NREAC.EQ.1) GO TO 95 000243
00302 960 N=0 000243
00303 970 CALL GOUTLINEACT,29) 000244
00304 980 CALL RDATA(1,N,990) 000250
00305 990 IF (N.LT.1 .OR. N.GT.NREAC) GO TO 90 000255
00307 1000 CONTINUE 000274
00310 1010 IF (IOPT.EQ.2) GO TO 200 000274
00310 1020 C 000274
00310 1030 C SELECT MODIFICATION OPTIONS 000274
00312 1040 CONTINUE 000277
00313 1050 CALL PAGIT 000277
00314 1060 NAST=1M 000300
00315 1070 IF (NAME(I,6).EQ.2M00) NAST=1M0 000302
00317 1080 ENCODE(102,1OUT,N,NAME(I,J),ANUM(I,J),J=1,5),PECT(I),MOLE(I), 000312
00317 1090 X ENTH(I),NAST,FAZ(I),RTEMP(I),FOR(I),DENS(I) 000312
00337 1100 CALL GOUTLINE1,125) 000313
00340 1110 CALL GOUTLINE2,119) 000317

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00040 1660 60 TO 100 000400
00040 1690 000460
00041 1700 000662
00042 1710 000662
00043 1720 000662
00044 1730 000672
00044 1740 000701
00044 1750 000701
00045 1760 000703
00046 1770 000703
00047 1780 000707
00052 1790 000717
00053 1800 000717
00054 1810 000720
00057 1820 000723
00061 1830 000723
00062 1840 000725
00063 1850 000727
00064 1860 000731
00065 1870 000733
00066 1880 000735
00067 1890 000737
00070 1900 000745
00072 1910 000745
00072 1920 000745
00072 1930 000745
00073 1940 000747
00074 1950 000747
00075 1960 000751
00076 1970 000752
00077 1980 000754
00500 1990 000770
00503 2000 000770
00504 2010 000775
00505 2020 001000
00506 2030 001003
00510 2040 001003
00511 2050 001015
00514 2060 001015
00515 2070 001023
00515 2080 001023
00516 2090 001023
00517 2100 001032
00521 2110 001032
00522 2120 001032
00523 2130 001036
00524 2140 001037
00525 2150 001046
00526 2160 001046
00527 2170 001051
00531 2180 001062
00532 2190 001062
00533 2200 001066
00534 2210 001067
00535 2220 001077
00537 2230 001110

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60 TO 100
 CONTINUE
 CALL DMRTF(EMP,24,DEMS(N),S)
 CALL PDATF(1,DEMS(N),S,10)
 GO TO 100

DELETE A REACTANT
 CONTINUE
 MREAC=MREAC-1
 DO 220 I=M,MREAC
 DO 210 J=1,6
 NAME(I,J)=NAME(I+1,J)
 AMUM(I,J)=AMUM(I+1,J)
 CONTINUE
 PECUT(I)=PECUT(I+1)
 MOLE(I)=MOLE(I+1)
 ENTAL(I)=ENTAL(I+1)
 FAZ(I)=FAZ(I+1)
 RTMP(I)=RTMP(I+1)
 FOR(I)=FOR(I+1)
 DEMS(I)=DEMS(I+1)
 CONTINUE
 GO TO 50

ADD A REACTANT
 CONTINUE
 MREAC=MREAC+1
 M=MREAC
 CALL GOUT(EMP,1A,66)
 CALL GOUT(EMP,10,98)
 DO 305 I=1,6
 J=I-1102+1
 RDM(J)=2M
 RDM(J+1)=0
 CONTINUE
 CALL PDATF(10,RDM,8300)
 DO 307 I=1,5
 J=I-1102+1
 FLD(10,36,NAME(M,I))=FLD(10,36,RDM(J))
 CALL CHECRNAME(M,I)
 AMUM(M,I)=RDM(J+1)
 CONTINUE
 CONTINUE
 CALL GOUT(EMP,2,36)
 PECUT(M)=0
 CALL PDATF(1,PECUT(M),8310)
 CONTINUE
 MOLE(M)=1M
 IF (ROVSEIEMP,20,301) MOLE(M)=1M
 CONTINUE
 CALL GOUT(EMP,3,50)
 ENTAL(M)=0
 CALL PDATF(1,ENTAL(M),8330)
 IF (ROVSEIEMP,3,421) NAME(M,6)=2M00
 CONTINUE

0412 101300

OPÉAO

00110	CALL GOUTTEMP(4,24)	00110
00111	FAZINI=1M5	00111
00112	CALL RDCMARIP(27(M),1,-1,5340)	00112
00113	CONTINUE	00113
00114	CALL GOUTTEMP(5,24)	00114
00115	PTEMPINI=0.	00115
00116	CALL RDATAF(1,RTEMPINI,8350)	00116
00117	CONTINUE	00117
00118	CALL GOUTTEMP(6,30)	00118
00119	FOR(I)=1M5	00119
00120	CALL RDCMARIP(OR(M),1,-1,5340)	00120
00121	CONTINUE	00121
00122	CALL GOUTTEMP(7,24)	00122
00123	DEMSINI=0.	00123
00124	CALL RDATAF(1,DEMSINI,8370)	00124
00125	GO TO %	00125
00126	C	00126
00127	C	00127
00128	STORE CASE TO FILE B	00128
00129	CONTINUE	00129
00130	REWIND IO	00130
00131	IF (IO.NE.M5) GO TO 400	00131
00132	DO 406 I=1,5	00132
00133	READ (IO) MOUNTY	00133
00134	CONTINUE	00134
00135	CONTINUE	00135
00136	WRITE (IC) MREAC,CF	00136
00137	DO 410 I=1,MREAC	00137
00138	WRITE (IO) (NAME(I),J),AMUM(I),J),J=1,5),PCUT(I),MOLE(I),	00138
00139	ENTH(I),NAME(I,6),AMUM(I,6),FAZ(I),RTEMP(I),FOR(I),DEMS(I))	00139
00140	CONTINUE	00140
00141	IF (IO.NE.M5) GO TO 420	00141
00142	IF (.NOT.ROVSI*TYPE YES TO EDIT COAL REACTANT DATA*,35))	00142
00143	GO TO 420	00143
00144	IO=M5	00144
00145	REWIND IO	00145
00146	DO 412 I=1,5	00146
00147	READ (IO) MOUNTY	00147
00148	CONTINUE	00148
00149	GO TO IO	00149
00150	ENDFILE IO	00150
00151	RETURN	00151
00152	002 FORMAT(12,2X,5(A2,F0.4,2X),F10.6,2X,A1,F15.4,A1,3X,A5,F12.3,	00152
00153	1 3I,A1,F12.5,1)	00153
00154	END	00154

END OF COMPILATION: NO DIAGNOSTICS.

June, 1945

SAVE

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AFOR,S SAVE,SAVE
MSA E3 -10/15/80-13:07:45 (13,)

SUBROUTINE SAVE ENTRY POINT 000501
NEWOF ENTRY POINT 000504

STORAGE USED: CODE(1) 000507; DATA(0) 000104; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 HOLCON 000010
0005 SPECES 017106
0006 MISC 001701
0007 INDX 000091
0010 C.C. 000003
0011 CFUEL 000004

EXTERNAL REFERENCES (BLOCK, NAME)

0012 H.CALC
0013 EXP
0014 MW0US
0015 M102S
0016 M101S
0017 MERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000137	100L	0001	000056	13L	0001	000042	1326	0001	000073	15L	0001	000112	20L
0001	000172	200L	0001	000161	2016	0001	000207	2106	0001	000326	2526	0001	000241	302L
0001	000335	3176	0001	000127	50L	0000	000014	730F	0000	000017	732F	0001	000318	744L
0001	000322	745L	0001	000356	750L	0001	000365	760L	0000	000035	770F	0000	000045	780F
0000	000050	785F	0005	011052	A	0006	000640	AM	0006	000705	AM1	0006	001135	ANUM
0003	000000	ATHN	0006	000004	ATOM	0006	000514	BO	0006	000545	BOF	0007	000036	ALCH
0011	R 000000	CF	0005	000000	COEF	0000	R 000006	COF	0007	000001	CONVG	0006	000706	CPR1
0006	000634	CPSUM	0006	000654	DATA	0005	010624	DELM	0010	000002	DFMAND	0006	001560	DENS
0005	R 004312	EN	0004	000000	END	0005	R 010150	EMLN	0006	R 001700	EMLSAV	0006	000000	ENN
0006	R 001676	ENHL	0006	R 001677	ENSAVE	0006	001414	ENTH	0006	R 000636	ERAT	0006	001445	FAZ
0000	R 000003	FAL	0000	R 000013	FF	0000	R 000002	FHH	0006	001527	FHX	0000	R 000001	FUU
0004	000001	GAS	0003	000001	GNET	0010	000000	GRAPH	0011	000001	HNVV	0007	000003	HP
0006	R 000642	HPP	0000	R 000012	HS	0006	R 000637	HSUBO	0005	010376	HO	0007	I 000030	IC
0007	000000	IDEBUG	0004	I 000002	IE	0007	000015	IMAT	0000	000057	INJPS	0007	L 000023	IONS
0007	000021	P	0007	I 000037	IQSAVE	0007	I 000016	IO1	0007	I 000005	ISV	0007	000034	IT
0005	I 016266	IUSE	0004	000003	IZERO	0000	I 000005	J	0007	I 000026	JLIQ	0010	I 000001	JOUT
0007	I 000025	JSOL	0007	000031	JS1	0007	000014	KMAT	0004	I 000004	LANK	0006	I 000463	LLMT
0000	I 000004	LL1	0007	I 000040	LSAVE	0004	000005	MOL	0007	000006	MOLES	0006	000707	NAME
0007	000024	NC	0007	000022	NEWIR	0007	000035	MFZ	0007	I 000012	NLM	0007	000017	NOF
0007	000020	NOMIT	0007	000007	NP	0007	I 000011	NPT	0007	000027	NREAC	0007	I 000013	NS
0000	I 000000	NSPP1	0007	000010	NT	0006	R 000635	OF	0004	000006	OX	0006	001644	OXF
0003	000002	PATH	0006	001363	PECVT	0011	R 000003	PER	0006	000633	PP	0003	R 000003	RBAR
0003	000004	RRR	0006	R 000644	RH	0006	R 701611	RHOP	0006	001612	RHW	0006	001476	RTFMP

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0003 000005 RVR 0005 000004 S 0007 000033 SHOCK 0005 R 016660 SUM 0007 000004 SP
0006 015364 SUB 0000 R 000007 SUM 0006 000001 SUM 0006 016819 TEMP
0006 000632 THIGH 0006 001643 TLM 0006 000630 TLOW 0006 000627 TM 0006 000631 TMIO
0007 000002 TP 0006 000002 TT 0006 R 000696 VMIN 0007 L 000032 VOL 0006 R 000650 VPLS
0000 R 000011 V1 0000 R 000010 V2 0011 R 000002 WCR 0006 000652 WP 0006 000007 ZERO

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SUBROUTINE SAVE
10 C
20 C
30 C SAVED OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES
40 C
50 COMMON /CONSTS/ ATNM GNET, PATM, BAR, RBR, RVR
60 COMMON /HOLCON/ EMO, GAS, IE, IZERO, LAMM, MOL, OX, ZERO
70 COMMON /SPECES/ CDEF(12, 7, 150), S(150), EN(150, 13), ENLM(150), MOL(150)
80 C 1, DELM(150), A(15, 150), SUB(150, 3), IUSE(150), TEMP(150, 2), SLM(150),
90 INCLUDE SPECES
100 COMMON /MISC/ ENM, SUMM, TT, SO, ATOM(13, 101), LLM(125), BD(125),
110 BOP(125, 2), TM, TLOW, TMIO, THIGH, PP, CP, SUM, OF, OPAT,
120 MSUBD, AM(12), HPP(12), RM(12), VMIN(2), VPLS(12), BP(12),
130 DATA(125), AMI, CPRI, NAME(125, 6), ANUM(125, 6), PECWT(125),
140 ENW(125), F(125), TEMP(125), FOX(125), DEN(125), RMOP,
150 RMV(125), TLM, OXE(126), ENML, ENSAVE, ENLSAV
160 COMMON /IMOX/ IDEBUG, CONVG, TP, MP, SP, ISV, MOLES, MP, NT, NPT, ML, MNS,
170 KMAT, IMAT, IOL, MOV, MOMIT, IP, NEUR, IONS, MC, JSOL, JLIQ,
180 NREAC, IC, JSI, VOL, SHOCK, IY, MFZ, CALCH, IOSAVE, LSARE
190 C
200 COMMON /CCC/ GRAPH, JOUT, DEMAND
210 COMMON /CFUEL/ CF, MHV, WCR, PER
220 C
230 DATA FUU/AMU, C, FMM/AMH, C, FCAL/QHAL/6/
240 LOGICAL CALCH, IONS, VOL
250 C
260 IF (ISV) 100, 10, 200
270 C NEXT POINT FIRST IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS Y
280 10 IOL = IOSAVE
290 ENM = ENSAVE
300 ENML = ENLSAV
310 LLI = MLM
320 DO 50 J = 1, NS
330 IF (I, MOT, IONS, OR, LLM(MLM), EQ, LSARE) 60 TO 15
340 IF (LLM(MLM), EQ, IE) 60 TO 13
350 IF (IUSE(J), NE, -10000) 60 TO 15
360 IUSE(J) = 0
370 LLI = MLM+1
380 GO TO 20
390 13 IF (SLM(J), ME, 0, OR, IUSE(J), ME, 0) 60 TO 15
400 LLI = MLM-1
410 IUSE(J) = -10000
420 GO TO 50
430 15 IF (IUSE(J), EQ, 0) 60 TO 20
440 EN (J, MPT) = SLM(J)
450 IF (IUSE(J), GT, 0) IUSE(J) = - IUSE(J)
460 IF (EN(J, NPT), GT, 0, 0) IUSE(J) = - IUSE(J)
470 GO TO 50

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OF POOR QUALITY

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00162 480 20 EN(J,MPT) = 0.
00163 490 EN(J,MPT) = SLN(J)
00164 500 IF (EN(J,MPT) + 10.50 .LE. ENML) GO TO 50
00166 510 EN(J,MPT) = EXP(ENML(J))
00167 520 50 CONTINUE
00171 530 NLN = LLJ
00172 540 RETURN
00173 550 C FIRST T-SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T
00174 560 100 ISV = -ISV
00175 570 10 SAVE = 101
00176 580 ENSAVE = ENM
00177 590 ENLSAV = ENML
00178 600 LSAVE = LLMT(MLM)
00179 610 DO 150 J = 1,MS
00180 620 SLN(J) = ENML(J)
00181 630 150 IF (IUSE(J) .NE. 0) SLN(J) = EN(J,ISV)
00182 640 C USE COMPOSITIONS FROM PREVIOUS POINT
00183 650 200 DO 300 J = 1,MS
00184 660 300 EN(J,MPT) = EN(J,ISV)
00185 670 RETURN
00186 680 C CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIO
00187 690 ENTRY NEWOF
00188 700 WRITE(JOUT,730) OF
00189 710 730 FORMAT(1HOF = ,F10.6)
00190 720 IF (CF+1.0) ,302,
00191 730 COF=OF/CF
00192 740 WRITE(JOUT,732) COF,WCR,PER
00193 750 732 FORMAT(12X,OXIDIZER/COAL= ,F6.4,OX, WATER/COAL= ,F6.4,
00194 760 X SX, CARBON CONVERSION= ,F8.4)
00195 770 302 CONTINUE
00196 780 SUM = OF + 1.
00197 790 V2 = (OF+VMIN(1)+VMIN(2))/SUM
00198 800 V1 = (OF+VPLS(1)+VPLS(2))/SUM
00199 810 IF (V2 .LT. 0.0) EQRT = ABS(V1)/V2)
00200 820 IF (RH(1) .GT. 0.0 .AND. RH(2) .GT. 0.0) GO TO 744
00201 830 RHOP = RH(2)
00202 840 IF (RHOP .LT. 0.0) RHOP = RH(1)
00203 850 GO TO 745
00204 860 744 RHOP = (OF+1.0+RH(1)+RH(2))/(RH(1)+ OF +RH(2))
00205 870 745 DO 747 J = 1,MLM
00206 880 747 BO(J) = (RO(J,2) + BO(J,1)+OF)/SUM
00207 890 MPT = 1
00208 900 IF (.NOT.CALCH) GO TO 750
00209 910 CALL MCALC
00210 920 CALCH = .FALSE.
00211 930 IF (OF .GT. 0.0) HPP(1) = SUM+HPP(1)/OF
00212 940 HPP(2) = SUM+HPP(2)
00213 950 GO TO 760
00214 960 750 HSUBO = (HPP(2) + HPP(1)+OF)/(HPP(1)+SUM)
00215 970 760 IC = 0
00216 980 JSOL = 0
00217 990 JLIO = 0
00218 1000 HS = PRAR+HSUBO
00219 1010 WRITE(JOUT,770)
00220 1020 770 FORMAT(1H,17X,WHFUEL ,13X,7HOXIDANT ,12X,7HMLXTURE
00221 1030 780 FORMAT(1H 2AN,3E18.8/)

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00300 1000
00301 1050
00302 1060
00303 1070
00304 1080
00305 1090
00306 1100
00307 1110

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FF = FMH
IF (VOLIFF = FMH)
  WRITE(JOUT,780) FF,FCAL ,MPP(1),MPP(2),MPP(3),MS
  WRITE(JOUT,785)
  785 FORMAT (1X,M KG-ATOMS/KG)
  WRITE(JOUT,780) (LLH(I),J),LANK,80(I,J,2),80(I,J,1),J = 1,M,M)
  RETURN
END

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END OF COMPILATION: NO DIAGNOSTICS.

2MOG.P SEARCH

FOR, S SEARCH, SEARCH

MSA E3 -10/15/80-13:07:40 (16,)

SUBROUTINE SEARCH ENTRY POINT 000000

STORAGE USED: CODE(11) 000001; DATA(10) 000121; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 HOLCOM 000010
 0004 SPECS 011106
 0005 MISC 001701
 0006 INDX 000001
 0007 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0010 MOVABS
 0011 HOLOIT
 0012 PAGIT
 0013 GOUT
 0014 MRENS
 0015 MRDUS
 0016 MIO2S
 0017 MIO1S
 0020 MWDUS
 0021 MERR3S

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000022	10F	0001	000021	1256	0001	000022	1306	0001	000310	1451	0001	000050	1456
0001	000102	154G	0001	000313	170L	0001	000126	1716	0001	000326	171L	0000	000045	172F
0001	000126	173G	0000	000055	176F	0000	000030	20F	0001	000144	2046	0001	000154	207G
0001	000204	220G	0001	000211	225G	0001	000222	2336	0001	000276	2546	0001	000346	277G
0001	000376	306G	0000	000020	SF	0001	000042	7L	0001	000167	805L	0001	000171	810L
0001	000225	820L	0001	000234	825L	0000	000032	871F	0004	R 011052	A	0005	000640	AM
0005	000703	PHI	0005	001135	ANUM	0005	000004	ATOM	0000	R 000001	B	0005	000514	BO
0005	000545	BOP	0006	000036	CALCH	0004	R 000000	COEF	0006	000001	CONVG	0005	000708	CPRI
0005	000634	CPSUM	0005	000654	DATA	0004	R 004312	DATE	0004	010624	DELM	0007	000002	DEMAND
0005	001360	UENS	0004	004312	EM	0003	I 000000	END	0004	010150	ENLM	0005	001700	ENLSAV
0005	000000	ENM	0005	001676	ENML	0003	I 001677	ENSAVE	0005	001414	ENTH	0005	000636	EGRAT
0005	001445	FAZ	0005	001527	FOX	0003	I 000001	SAS	0007	000000	GRAPH	0006	000003	HP
0005	000642	HPP	0005	000637	MSUBO	0004	D10376	HO	0000	I 000013	I	0006	000030	IC
0006	000000	IDEBUG	0003	000002	IE	0006	000015	IMAT	0000	000073	INJPS	0006	000023	IONS
0006	000021	IP	0006	000037	IOSAVE	0006	000016	LOI	0006	000005	ISV	0006	000034	IT
0006	I 016266	IUSE	0000	I 000012	IX	0003	000003	IZERMO	0000	I 000014	J	0006	000026	JL10
0007	I 000001	JOUT	0006	000025	J50L	0006	000031	J51	0000	I 000017	K	0006	000014	KMAT
0006	I 000012	L	0003	000004	LANK	0005	I 000463	LLMT	0006	000040	LSAVE	0003	000005	MOL
0006	000006	MOLFS	0000	I 000005	MY	0005	000707	NAME	0006	I 000024	NC	0006	L 000022	NEUR
0006	000035	NFZ	0006	000017	NOF	0006	I 000020	NOMT1	0006	000007	NP	0006	000011	NPT
0006	000027	NREAC	0006	I 000013	NS	0000	I 000000	NSPPI	0006	000010	MT	0005	000635	OF
0006	I 010150	O-MY	0003	000006	OX	0005	001644	OYF	0005	001363	PFCMT	0000	I 000011	PMA2

SEARCH

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0005 000633 PP 0005 000633 RH 0005 001611 ROP 0005 001612 RMW 0005 001976 RTEMP
0005 000664 S 0006 000633 SHOCK 0004 001660 SLM 0006 000004 SP 0005 015364 SUB
0005 000001 SUMW 0005 000003 SO 0004 0016514 TEMP 0005 000000 TLM
0005 R 000630 TLOW 0005 000627 TM 0005 R 000631 TMID 0006 000002 TP 0005 000000 TY
0000 P 000015 T1 0000 P 000016 T2 0005 000646 VMIN 0006 000032 VOL 0005 000680 VPLS
0005 000652 WP 0003 000007 ZERO
    
```

```

SUBROUTINE SEARCH
C SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED
COMMON /HOLCON/ EMO,GAS,IE,IZERO,LANW,MOL,OX,ZERO
COMMON/SPEC/ COEF(2,7,150),S(150),EM(150,13),ENL(150),MO(,50)
C 1 .DELM(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2),SLM(150)
INCLUDE SPECPR
COMMON /MISC/ ENM,SUMN,TY,SO,ATOM(3,101),LLMT(25),BO(25),
1 BOPI(25,2),TM,TLOW,THID,TWIGH,PP,CPSUM,OF,ORAT,
2 HSUBO,AM(2),MPP(2),RH(2),VMIN(2),VPLS(2),BP(2),
3 DATA(25),AM1,CPRI,NAME(25,6),ANUM(25,6),PECWT(25),
4 ENT(25),FAZI(25),RTEMP(25),F0(25),DEWS(25),RHOF,
5 RMV(25),TLM,OXE(26),ENML,EMSAVE,EMLSAV
COMMON /IMOX/ IOCBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,MT,MPT,L,MS,
1 KMAT,THAT,IQI,MOF,NOMIT,IP,MEWR,IONS,MC,JSOL,JLTO,
2 MREAC,IC,JSI,VOL,SHOCK,IT,MFZ,CALCH,IOSAVE,LSAVE
COMMON /CCC/ GRAPH,JOUT,DEMAND
C
C DIMENSION B(4),DATE(2,3),MT(4),OMIT(3,3)
EQUIVALENCE (DATE,EN),IEMLM,OMIT)
INTEGER EMO,GAS,OMIT,PHAZ,SUB
LOGICAL MEWR
C
C CHANGE WHEN CHANGE SPECIES SIZE
NSPPI=150
NCE=0
IX=0
SUM(1,1)=END
REWIND 4
DO 3 I=1,150
DO 3 J=1,L
DO 3 J=1,L
3 ATJ,I)=0.0
RAD(4,5) TLOW,THID,TWIGH
5 FORMAT (3F10.3)
MS=1
7 READ (9,10)SUB(INS,I),I=1,3),DATE(1,MS),DATE(2,MS),MT(J),R(J),
1 J=1,4),PHAZ,T1,T2
10 FORMAT(3A4,6A,2A3,4A2,F3.0),A1,2F10.3)
IF(SUB(INS,I),FO,END) GO TO 171
READ (4,20) I(COEF(I,J,MS),J=1,7),I=1,2)
20 FORMAT (5E15.8)
IF(NOMIT,FO,0) GO TO 810
DO 805 I=1,NOMIT
DO 804 J=1,3
    
```

SEARCH

```

00211 470 804 IF (OMIT(J,1)) .NE. SUB(NS,J)) 60 TO 805
00214 480 GO TO 7
00215 490 805 CONTINUE
00217 500 810 DO 820 K=1,N
00222 510 IF (R(K).EQ.0.) 60 TO 825
00224 520 DO 168 I=1,L
00227 530 168 IF (LLMT(I)) .EQ. MY(M)) 60 TO 820
00232 540 DO 819 J=1,L
00233 550 819 A(I,NS) = 0.
00237 560 GO TO 7
00240 570 820 A(I,NS) = 8(M)
00242 580 825 IUSE(NS) = 0
00243 590 IF (PHAZ.EQ.6AS) 60 TO 170
00245 600 NC = NC+1
00246 610 TEMP(MC,1) = T1
00247 620 TEMP(MC,2) = T2
00250 630 IX = IX+1
00251 640 IF (IUSE(NS-1).EQ.0. .OR. MC.EQ.1) 60 TO 145
00253 650 DO 830 I=1,L
00256 660 830 IF (A(I,NS)) .NE. A(I,NS-1)) 60 TO 145
00261 670 IX = IX-1
00262 680 145 IUSE(NS) = -IX
00263 690 170 NS = NS+1
00264 700 IF (NS.LE.NSPEC) 60 TO 7
00266 710 WRITE (JOUT,871)
00270 720 871 FORMAT (/20X,5#DIMENSIONS IN /SPECES/ FOUND TO BE TOO SMALL IN S
00271 730 1EARCH/)
00272 740 171 NS = NS-1
00273 750 NEWR = .FALSE.
00275 760 WRITE (JOUT,172)
00276 770 172 FORMAT(42#SPECIES BEING CONSIDERED IN THIS SYSTEM )
00301 780 DO 174 I=1,NS,5
00302 790 K = I + 4
00304 800 IF (NS .LT. K) K = NS
00304 810 174 WRITE (JOUT,176) (DATE(I,J),SUB(J,1),SUB(J,2),SUB(J,3),
00304 820 1 J=1,K)
00317 830 176 FORMAT(5F,2A3,2X,3A4)
00320 840 CALL MOVABS(500,50)
00321 850 CALL HOLDIT
00322 860 CALL PAGEIT
00323 870 CALL GOUT(' ',1)
00324 880 RETURN
00325 890 END

```

END OF COMPILATION: NO DIAGNOSTICS.

END OF P. SMCR

SMCM

AFOR, S SMCN, SMC
MSA E3 -10/15/80-13:07:51 (12,)

SUBROUTINE SMCM ENTRY POINT 001367

STORAGE USED: CODE(1) 001401: DATA(0) 000263: BLANK COMMON(12) 000000

COMMON BLOCKS:

0003 CONSTS 000006
0004 MOLCOM 000010
0005 POINTS 000335
0006 SPECES 017106
0007 MISC 001701
0010 DOUBLE 001560
0011 INDX 000041
0012 PERF 000166
0013 OUPY 000073
0014 CCC 000003

EXTERNAL REFERENCES (BLOCK, NAME)

0015 ROYES
0016 PAGIT
0017 CHR512
0020 GOUT
0021 MEMOF
0022 HCALC
0023 OUT1
0024 OUT2
0025 EOLBRM
0026 SAVE
0027 OUT3
0030 NNNLS
0031 NNNLS
0032 MUDUS
0033 N1028
0034 SORT
0035 N1038
0036 N1018
0037 ALO6
0040 EXP
0041 MEMR35

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	0001	000211	14L	000011	1456	0001	000221	15L	0001	001001	150L
0000	0001	000022	156G	000101	16F	0001	001112	163L	0001	000126	17L
0001	0001	000073	204G	000114	21L	0001	000136	2236	0001	000147	2316
0001	0001	000356	3236	0001	000376	3346	0001	000520	3416	0001	000539
0001	0001	000320	44L	0001	000325	45L	0000	000137	46F	0001	001057
0001	0001	000547	50L	0001	001201	520G	0001	001232	536G	0001	001247
0001	0001	000512	47L								5476

SMCH

0001	001266	561G	0001	001303	5726	0000	000176	58F	0001	001322	6046	0001	001345	6206
0000	000266	68F	0001	000750	75L	0000	000111	66F	0000	000122	662F	0000	000131	663F
0001	001106	880	0006	011052	A	0007	000111	AM	0007	000705	AM1	0007	001135	ANUM
0003	000000	ATM	0007	000004	ATM	0000	000036	AX	0000	000037	AXX	0000	000020	A1
0005	000018	BQ	0007	000545	BOF	0011	000036	CALCH	0006	000000	COEF	0000	000001	CONV6
0005	000032	CPR	0007	000706	CPR1	0007	000634	EPSUM	0007	000654	DATA	0006	010426	DELM
0014	000000	DEMAND	0007	001560	DEMS	0005	000064	DLVPT	0005	000047	DLVTP	0006	004312	EN
0004	000000	END	0006	001030	EMLM	0007	001780	EMLSAV	0007	000000	ELM	0007	001476	ENML
0007	001677	ENSAVE	0006	001414	ENTH	0012	000165	EOL	0007	000636	EORAT	0013	000002	FA
0013	000003	FAP	0007	001445	FAZ	0013	000005	FB	0013	000006	FC	0013	000007	FCE
0013	000012	FCST	0013	000014	FV	0013	000015	F8	0013	000017	F8E	0013	000020	F6V
0013	000021	FM	0013	000023	FM	0013	000025	PIV	0013	000027	FM	0000	000001	FMM
0013	000031	FMT	0013	000030	FM	0013	000032	FOUR	0007	001527	F8X	0013	000053	FP
0009	000002	FPP	0000	000003	FRA	0000	000004	F8	0013	000054	FS	0013	000056	F5V
0013	000057	FT	0013	000061	FTK	0000	000005	FTT	0000	000006	FU1	0000	000007	FU2
0013	000063	FV	0013	000065	FVEL	0000	000006	FV21	0000	000011	FV22	0000	000012	FV23
0013	000001	F13	0013	000000	F9X	0010	000000	G	0005	000101	GAMMAS	0000	000020	GAMMA1
0003	000001	BAS	0010	001316	GG	0003	000001	GNET	0014	000000	GRAPH	0011	000003	MP
0007	000042	HPP	0000	000030	HS	0007	000637	MSUM	0005	000000	MSUM	0006	010376	MB
0000	000022	I	0011	000030	IC	0011	000000	IDEBUG	0004	000002	IE	0011	000015	IMAT
0000	000013	INCOE0	0000	000014	INCOF2	0000	000233	INJPS	0000	000021	ISF	0011	000023	IOWS
0011	000021	IP	0011	000037	IQSAVE	0011	000036	IQ1	0011	000005	ISV	0011	000034	IT
0006	016266	IUSE	0004	000003	IZERO	0000	000025	J	0011	000726	KL10	0014	000001	JOUT
0011	000025	JSQL	0011	000031	J51	0000	000000	K	0011	000014	KMAT	0000	000004	LAMH
0007	000043	LMT	0011	000040	LSAVE	0012	000116	MACH1	0004	000005	MOL	0011	000006	MOLES
0000	000017	MU12RY	0000	000016	M1	0012	000150	M2M1	0007	000707	NAME	0011	000024	MC
0011	000022	NEWR	0011	000035	NFZ	0011	000012	NLM	0011	000017	NOF	0011	000020	NOH1T
0011	000007	NP	0011	000011	NPT	0011	000027	NREAC	0011	000013	NS	0000	000023	NSK
0000	000000	NSPP1	0011	000010	NT	0007	000635	OF	0013	000067	OME	0004	000006	OX
0007	001644	OXF	0005	000116	P	0003	000002	PATH	0012	000000	PCP	0007	001343	PECM1
0007	000633	PP	0005	000217	PPP	0000	000026	PI	0000	000031	P21	0000	000033	P21L
0003	000035	RBAR	0003	000004	RBR	0015	000000	RDYES	0007	000644	RM	0007	001611	RMOP
0000	000035	RM012	0007	001612	RMV	0012	000133	RRMO	0007	001476	RTEMP	0003	000005	RVR
0006	004044	S	0000	000035	SEOL	0000	000041	SHKIMP	0011	000033	SHOCK	0006	014400	SLM
0005	000251	SONVEL	0011	000004	SP	0005	000015	SSUM	0006	015364	SUB	0007	000001	SUMH
0007	000003	SD	0003	000130	T	0006	016514	TEMP	0007	000032	TM16H	0013	000070	THREE
0007	001643	TEN	0007	000430	TLOW	0007	000627	TM	0007	000631	TM10	0005	000320	TOTM
0011	000002	TP	0007	000002	T1	0005	000266	T1T	0013	000071	TW0	0000	000027	T1
0012	000007	T2T1	0000	000032	T21	0000	000034	T21L	0005	000303	UTW0	0012	000101	U1
0012	000064	U1U2	0005	000202	V	0007	000646	VMIM	0012	000032	VMOC	0011	000032	VOL
0007	000650	VPLS	0005	000234	WM	0007	000652	WP	0010	001510	X	0004	000007	ZERO
0013	000072	ZEROF												

00101	10	SUBROUTINE	SMCH	COMMON /CONSTS/	ATM, GNET, PATH, RBAR, RBR, RVR	/CONSTS/
00101	20			COMMON /HOLCON/	END, GAS, IE, IZERO, LANK, MOL, OX, ZERO	/HOLCON/
00103	30			COMMON/POINTS/H2SUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)		
00105	50			1 GAMMA(13), PT(26), T(26), V(13), P(13), SONVEL(13), TTT(13)		
00105	60			2 UTWC(13), TOTM(13)		
00105	70			COMMON/SPECES/COEF(12, 7, 150), S(150), EN(150, 13), ENLM(150), MO(150)		
00105	80			1 DELM(150), A(15, 150), SUB(150, 3), TUSE(150), TEMPI(50, 2), SLM(150)		
00105	90			INCLUDE SPECIM		
00106	100					

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00112 COMMON /MISC/ MM,SUMN,TT,SO,ATOM(3,101),LLMT(25),BO(125),
00113 BO(125,21),TH,TLOW,IMID,TWIGH,PP,CP,SM,OF,EGRAT,
00114 MSUBO,AM(2),MPP(2),MM(2),VM(2),VPLS(2),MP(2),
00115 DATA(25),AM1,CPM1,NAME(25,6),ANUM(25,6),PECUT(25),
00116 ENH(25),FZ(25),RYEMP(25),FOX(25),DEMS(25),AMOP,
00117 RM(25),TLM,OXE(26),ENML,ENSAVE,ENLSAV
00118 COMMON /DOUBLE/ G120,21, X1201
00119 COMMON /INDEX/ IDEBUG,CONVG,TP,MP,SP,ISV,MOLES,MP,NT,MPT,MLM,MS,
00120 KMAT,IMAT,IOI,NOF,NOMIT,IP,NEUR,IONS,MC,JSOL,JLIG,
00121 NREAC,IC,JSI,VOL,SHOCK,IT,MFZ,CALCM,IOSAVE,LSAVE
00122 COMMON /PERF/ PCP(26),VMOC(13),T2(1,13),UIU2(13),UI(13),
00123 MAC(113),ARMQ(13),M2M(13),EOL
00124 COMMON /OUP/ F0X,F13,FA,FAPI(2),FB,FC,FCPI(3),FCST(2),FCV,FE(2),
00125 FCE,F6V,FM(2),FI(2),FIV(2),FM(2),FMT(15),FM(2),FOUR,
00126 FP,FS(2),FSV,FT(2),FTK(2),FV(2),FVEL(2),ONE,THREE,
00127 TWO,ZERO
00128 COMMON /CCC/ GRAPH,JOUT,DEMAND
00129 DATA FMH/6MM2/M1 /,FPP/6MP2/P1 /,FPA/6MRO2/R/,FRB/6MM01 /,
00130 FTT/6MP2/P1 /,FU1/6MU1 VE/,FU2/6MU2 VE/,FV21/6W21U1-/ ,
00131 FV22/6MU2/M/5/ FV23/2MEC/
00132 DOUBLE PRECISION G,GG,X
00133 EQU,VALENCE (X(9),GG)
00134 LOGICAL EOL,INCODE0,INCODE2,SEOL,TP
00135 LOGICAL ROYES
00136 REAL M1,MACH1,M2M1,MU12M1
00137 NAMELIST /SMKINP/ GAMMA1,INCODE0,INCODE2,MACH1,U1
00138 /SHKINP/
00139 IOF = 0
00140 TP=.TRUE.
00141 CPM1 = 0.
00142 DO 10 I=1,13
00143 MACH1(I)=0.
00144 U1(I) = 0.0
00145 GAMMA1 = 0.
00146 INCODE0 = .TRUE.
00147 INCODE2 = .TRUE.
00148 DO 10 I = 1,INREAC
00149 NAME1(I,6)=IZERO
00150 CALL PAGIT
00151 CALL CMRSIZ(1)
00152 IF IRYTES(I,TYPE YES FOR PRESENT VALUES OF SHKINP NAMELIST',46))
00153 WRITE(6,SHKINP)
00154 CALL CMRSIZ(1)
00155 CALL GOUT(I,TYPE NAMELIST SHKINP HERE',21)
00156 READ (5,SHKINP)
00157 WRITE(JOUT,SHKINP)
00158 SEOL = INCODE0
00159 IF (I(1) .LE. 0.0) T(1) = PTEMP(1)
00160 DO 20 I = 1,13
00161 IF (MACH1(I) .LE. 0.0 .AND. U1(I) .LE. 0.0) GO TO 21
00162 NMX = 1
00163

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SMCM

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00363 1230 NP1 = 1
00364 1200 07 GAMMA1 = GAMMA5(NP1)
00365 1250 MI = UM(NP1)
00366 1200 P1 = PPP(NP1)
00367 1270 T1 = TTT(NP1)
00368 1200 MS = MSUM(NP1)
00369 1200 P21 = (2.0 * GAMMA1 * MI * T1) / (GAMMA1 * P1)
00370 1300 T21 = (2.0 * GAMMA1 * MI * T1) / (GAMMA1 * P1)
00371 1310 IF (T1 * T21) .GT. 2000. AND. EQL T21 = .7 * T21 + 600. / T1
00372 1320 MU12RT = MI * U1(NP1) * 0.2 / (INBRT1)
00373 1330 P21L = ALOG(P21)
00374 1340 T21L = ALOG(T21)
00375 1350 DO 100 I = 1, 4
00376 1360 T1 = T21 * T1
00377 1370 PP = P21 * P1
00378 1380 IF (.NOT. EQL) GO TO 80
00379 1390 CALL ZOLDRM
00380 1400 GO TO 50
00381 1410 C FROZEN
00382 1420 80 TLM = ALOG (T1)
00383 1430 CALL MCALC
00384 1440 MSUM(NP1) = MSUBO
00385 1450 CPRINT1 = CPR
00386 1460 50 MU012 = MU12RT / (UM(NP1) * P21)
00387 1470 GG = MU012 * MU12RT
00388 1480 G1,11 = -GG * OLVP(NP1)
00389 1490 G1,21 = -GG * OLVP(NP1)
00390 1500 G1,31 = P21 - 1.0 * MU12RT * (MU012 - 1.0)
00391 1510 GG = (U1(NP1) * MU012) * 0.2 / (MR
00392 1520 G2,11 = -GG * OLVP(NP1)
00393 1530 G2,21 = -GG * OLVP(NP1)
00394 1540 G2,31 = MSUM(NP1) - MS - U1(NP1) * 0.2 / (1.0 - MU012 * 0.2 / (1.0 * MR
00395 1550 X11 = G1,11 * G1,21 - G1,21 * G1,11
00396 1560 X11 = (G1,11 * G1,21 - G1,21 * G1,11) / X13
00397 1570 X12 = (G1,11 * G1,21 - G1,21 * G1,11) / X13
00398 1580 AX = X11
00399 1590 AX = X12
00400 1600 IF (AX * LT. 0.1) AX = -AX
00401 1610 IF (AX * LT. 0.1) AX = -AX
00402 1620 IF (AX * GT. 0.1) AX = AX
00403 1630 IF (AX * LT. 0.0005) GO TO 150
00404 1640 AX = AX / 0.050652
00405 1650 IF (AX * LE. 1.1) GO TO 75
00406 1660 X11 = X11 / AX
00407 1670 X12 = X12 / AX
00408 1680 75 P21L = P21L * X11
00409 1690 T21L = T21L * X12
00410 1700 P21 = EXP(P21L)
00411 1710 T21 = EXP(T21L)
00412 1720 100 WRITE (JOUT, 125) U1(NP1)
00413 1730 125 FORMAT (25H) NO CONVERGE FOR U1 = .F0.2.66H ANSWERS PROBABLY NO
00414 1740 150 IF (RELIABLE, SOLUTION PROBABLY DOES NOT EXIST)
00415 1750 150 MU012 = 1.0 / MU012
00416 1760 MU12RT = MU12RT / MU1
00417 1770 CPRINT1 = P21
00418 1780 T21(NP1) = T21
00419 1790 30000

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SNCH

DATE 101500 PAGE 6

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00445 1700 IF (MPT) .GE. IDEBUG .AND. IDEBUG .NE. 0) WRITE(JOUT,152) I,721.021
00453 1800 152 FORMAT(10,0,10 NO.=,11,78,7M2/11 =,F9.2,7H,7M2/P1 =,F9.2 )
00454 1810 U10(MPT) = U1(MPT)*RHO12
00455 1820 U102(MPT) = U1(MPT)-U10(MPT)
00456 1830 IF (.NOT.EQ.) GO TO 161
00460 1840 DO 800 N=1,NS
00463 1850 IF (USE(R1,1,0)) GO TO 800
00465 1860 IF (MLMIN).GT.-87..AND.EMLN(K).LT.87.) ENIN,MPT, = EXP1EMLN(K))
00467 1870 800 CONTINUE
00471 1880 GO TO 431
00472 1890 C FROZEN
00473 1900 161 PR(MPT) = DP
00474 1910 Y1(MPT) = Y
00475 1920 GMM2(MPT) = CPRINT/(Cp(MPT) - 1.0/AM1)
00476 1930 431 ISV = 0
00477 1940 IF (MPT.LT.NSH) ISV=MPT
00478 1950 IF (MPT.EQ.1) ISV=-1
00479 1960 MPT = MPT+1
00480 1970 IF (EQ1) CALL SAVE
00481 1980 IF (MPT.LE.NSH) GO TO 47
00482 1990 MPT = NSH
00483 2000 C OUTPUT--2ND CONDITION
00484 2010 WRITE(JOUT,50)
00485 2020 50 FORMAT(11H,SHOCKED GAS (21) )
00486 2030 FM1(4) = TWO
00487 2040 WRITE(JOUT,FMT) FV2,FVEL,(UTWO(J),J = 1,MPT)
00488 2050 CALL OUT2
00489 2060 WRITE(JOUT,60)
00490 2070 60 FORMAT(26H,INCIDENT SHOCK PARAMETERS )
00491 2080 FM1(5) = THREE
00492 2090 WRITE(JOUT,FMT) FPP,FP,FB,(PCPI(J),J = 1,MPT)
00493 2100 WRITE(JOUT,FMT) FTT,FB,FB,(T2T1(J),J = 1,MPT)
00494 2110 FMT(4) = FOUR
00495 2120 WRITE(JOUT,FMT) FMM,FB,FB,(M1M1(J),J = 1,MPT)
00496 2130 WRITE(JOUT,FMT) FRR,FB,FB,(RMMO(J),J = 1,MPT)
00497 2140 FM1(2) = TWO
00498 2150 WRITE(JOUT,FMT) FV2,FV22,FV23,(U102(J),J = 1,MPT)
00499 2160 CALL OUT3
00500 2170 INCDEB = .FALSE.
00501 2180 IF (INCDEB .AND. EQ1) GO TO 17
00502 2190 IF (IOP.LT.NOP) GO TO 21
00503 2200 IP = .FALSE.
00504 2210 DO 999 K = 1,NREAC
00505 2220 999 RT(MPT) = T11
00506 2230 RETURN
00507 2240 END

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END OF COMPILATION: NO DIAGNOSTICS.

AM08.P THERM

THEMP

DATE 101500

PAGE

1

2FOR.S THERMP THERMP
MSA E3 -10/15/00-13:07:55 (19.1)

SUBROUTINE THERMP ENTRY POINT 000027

STORAGE USED: CODE(1) 000037; GATAID 000117; BLANK COMMON(2) 000000

COMMON BLOCKS:

0003 CONSIS 000006
0004 POINTS 000115
0005 MISC 001701
0006 INOR 000001
0007 OUPY 000073
0010 CCC 000003
0011 CFUEL 000002

EXTERNAL REFERENCES (BLOCK, NAME)

0012 M200Y
0013 EQLQHM
0014 NOVARS
0015 MOLDIT
0016 PAG
0017 GOUT
0020 OUT1
0021 OUT2
0022 OUT3
0023 GUT4
0024 SAVE
0025 MUDUS
0026 MIO26
0027 MIO18
0030 MERRIS

ORIGINAL PAGE IS
OF POOR QUALITY

STORAGE ASSIGNMENT (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000021	107	0000	000025	11F	0000	000033	12E	0001	00022	1258	000044	1326
0000	000041	207	0000	000045	21F	0000	000054	22F	0001	00034	2256	000261	2416
0000	000006	5F	0001	000061	000L	0001	000111	060L	0001	000162	061L	000207	062L
0000	000002	063F	0001	000265	064L	0000	000070	060F	0001	000359	070L	000003	071L
0001	000276	002L	0001	000006	05L	0003	000640	AM	0005	000705	AM1	00005	001135
0003	000000	AIMM	0005	000009	ATCM	0005	000514	00	0005	000545	00P	00004	000036
0011	000000	CF	0006	000001	COMVB	0004	000032	CPR	0005	000706	CPR1	00005	000034
0005	000034	DATA	0010	000002	DEMAND	0005	001540	DEMS	0004	000044	DLVPT	0004	000047
0005	001700	EMLSAV	0005	000000	EMM	0005	001676	EMCL	0005	001677	EMSAVE	0005	001910
0005	000036	EGRAY	0007	000002	FA	0007	000003	FAP	0005	001945	FAP	0007	000005
0007	000006	FC	0007	000007	FCP	0007	000012	FCSY	0007	000014	FCV	0007	000015
0007	000017	FGE	0007	000020	F6V	0007	000021	FM	0007	000023	F1	0007	000025
0007	000027	FM	0007	000031	FMT	0007	000050	FM	0007	000052	FOUM	0005	001327
0007	000053	FF	0007	000054	FS	0007	000056	FSV	0007	000057	FT	0007	000061
0000	000000	FUA	0000	000001	FUB	0007	000063	FV	0007	000065	FVEL	0007	000001

```

0007 C 00000 FX 0005 000101 GAMMAS 0003 000001 GHET 0000 000000 GRAPH 0011 000001 MHVV
0006 L 000003 HP 0005 000642 HPP 0005 R 000637 MSUBO 0004 000000 HSUM 0000 I 000003 I
0006 000030 IC 0006 I 000000 IOEBUG 0006 000015 IMAT 0000 000100 INJPS 0000 I 000002 IOF
0006 000023 IONS 0006 I 000021 IP 0006 000037 IOSAVE 0006 000016 IOI 0006 I 000005 ISV
0006 I 000034 IT 0006 000026 JLIO 0010 I 000001 JOUT 0006 000025 JSOL 0006 000031 JSI
0006 000014 KHAT 0005 000643 LLMT 0006 000000 LSAVE 0006 000006 MOLES 0005 000707 NAME
0006 000024 NC 0006 000035 NEUR 0006 000035 NZ 0006 000012 NLM 0006 I 000017 NOF
0006 000020 NOHIT 0006 I 000037 NP 0006 000011 NPT 0006 000027 NREAC 0006 000013 NS
0006 I 000010 NT 0005 R 000635 OF 0007 R 000637 ONE 0005 R 001644 OF 0004 R 00116 P
0003 000002 PATH 0005 001363 PECMT 0005 R 000633 PP 0004 000217 PPP 0003 R 000003 REAR
0003 000004 RBR 0005 000644 RH 0005 001611 RHOP 0004 001612 RMJ 0005 001476 RTEMP
0003 000005 RV9 0006 000033 SHOX 0004 000251 SONVEL 0004 L 000004 SP 0004 000015 SSUM
0005 000001 SUM 0005 000030 SO 0004 R 000150 T 0005 000632 TMIGH 0007 000070 THREE
0005 001643 TLM 0005 000630 TLOW 0004 000627 TM 0005 000631 TMID 0004 000320 TOTN
0006 L 000002 TP 0005 R 000002 TT 0004 000266 TTT 0007 R 000071 TWO 0004 R 000202 V
0004 R 000103 VM 0005 000646 VMIM 0004 000632 VOL 0008 000650 VPLS 0004 000234 VM
0005 000652 W 0007 000072 ZERO

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00101 1* C SUBROUTINE THERMP 000000
00101 2* C 000000
00103 3* COMMON /CONST/ ATMN, GNEI, P, IM, PGAR, RBR, RVR 000000
00104 4* COMMON /POINTS/ MSUM(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13) 000000
00104 5* 1, GAMMAS(13), P(26), V(13), PPP(13), VM(13), SONVEL(13), TTT(13) 000000
00104 6* 2, VLM(13), TOTN(13) 000000
00105 7* COMMON /MISC/ ENNI, SUMN, TT, SO, ATOM(13, 101), LLMT(25), BO(25), 000000
00105 8* 1, BO(25, 2), IM, TLOW, TMID, TMIGH, PP, CPSUM, OF, EORAT, 000000
00105 9* 2, MSUBO, AM(12), MPP(12), RH(12), VM(12), VPLS(12), MP(12), 000000
00105 10* 3, DATA(25), AMI, CPRI, NAME(25, 6), ANUM(25, 6), PECMT(25), 000000
00105 11* 4, ENTH(25), FAZ(25), RTEMP(25), FOX(25), DENSI(25), RHOP, 000000
00105 12* 5, RM(25), TLM, OXF(26), ENNL, ENSAVE, ENLSAV 000000
00106 13* COMMON /INDX/ IDEBUG, CONV6, TP, HP, SP, ISV, MOLES, NP, MT, NPT, NLM, NS, 000000
00106 14* 1, KHAT, IMAT, IOI, NOF, NOHIT, IP, NEUR, IONS, NC, JSOL, JLIO, 000000
00106 15* 2, NREAC, IC, JSI, YOL, SHOCK, I, I, NEZ, CALCH, IOSAVE, LSAVE 000000
00107 16* COMMON /OUP/ F9X, F13, FA, FAP(12), FB, FC, FCP(13), FCT(12), FCV, FE(12), 000000
00107 17* 1, FGE, FGV, FM(12), FI(2), FIV(2), FMT(15), FM(15), FOUR, 000000
00107 18* 2, FPA, FS(12), FSV, FT(12), FTK(12), FV(12), FVEL(12), ONE, THREE, 000000
00107 19* 3, TWO, ZERO 000000
00107 20* C 000000
00110 21* COMMON /CCC/ GRAPH, JOUT, DEMAND 000000
00110 22* C 000000
00111 23* COMMON /CFUEL/CF, MHVV 000000
00112 24* DATA FUA/GHU CAL//, FUB/GHGRAM / 000000
00113 25* LOGICAL HP, SP, TP, VOL 000000
00115 26* C 000000
00116 27* IF (T(1)) .LE. 0.01 T(1) = 3800.0 000000
00120 28* IOF = 0 000004
00121 29* 95 IOF = IOF+1 000006
00122 30* OF = OF+IOF 000011
00123 31* CALL NEWOF 000013
00123 32* SET ASSIGNED P OR VOLUME 000013
00124 33* DO 6/1 IP = 1, NP 000015
00124 34* PD = P(IP) 000035
00127 35* VLY(NPT) = P(IP) 000037

```


DATE 101580 PAGE 4

THE AMP

Address	Instruction	Hex	Dec
00270	92*		000352
00271	93*		000354
00272	94*		000356
00273	95*		000362
00274	96*		000373
00275	97*		000376
00276	98*		000403
00277	99*		000410
00278	100*		000436

END OF COMPILATION: NO DIAGNOSTICS.

ANDRE, P. VARENT

DATE 101580

VARFMT

00141	24*	IF (VII) .GE. 1.0E6) FMT(15) = PZERO	000071
00143	25*	45 CONTINUE	000102
00145	26*	RETURN	000102
00146	27*	END	000123

END OF COMPILATION: NO DIAGNOSTICS.

END IGNORED - IN CONTROL MODE

FIN

VARFMT

DATE 101500

PAGE

3

RUNID: LEWIST ACCT: JHPA01RS0021 PROJECT: SEVIGNOIN200

LOAD 15753 11/0 PUR -1 LEWIST

TIME: SUPS: 00:02:51.912 CRSUPS: 057007923

PU: 00:00:38.729 I/O: 00:01:29.681

CC/ER: 00:00:43.501 WAIT: 00:00:00.065

IMAGES READ: 61 PAGES: 118

START: 13:04:46 OCT 15.1980 FIN: 13:00:01 OCT 15.1980

THE 1108 (HOST2) WILL BE POWERED OFF NO LATER THAN NOV 15 1980

END OF PAGE 3
OF YOUR QUALITY

APPENDIX C
DOCUMENTATION CHECKLIST

DOCUMENTATION CHECKLIST

	Required	Completed	If not contained herein can be found in:
1. Title Page	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
2. Table of Contents	<input type="checkbox"/>	<input checked="" type="checkbox"/>	
3. Abstract	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
4. Introduction			
a. Objective or Purpose		<input checked="" type="checkbox"/>	
b. MSFC Form 3559	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
c. Background		<input checked="" type="checkbox"/>	
d. Related			
5. Problem Task Description	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
6. Method of Solution	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
7. Program Description			
a. Operating Environment			
(1) Hardware			
(a) Computer	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
(b) Core Requirement			
(c) Magnetic Tapes			
(d) Card Punch			
(e) Plotter			
(f) Drum/Disc			
(g) Other			
(2) Software			
(a) Operating System	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
(b) Programming Language(s)	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
(c) Type of Run			
(d) Library Subroutines ..	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	
b. Program Specifications			
c. Subroutines or Subprograms			
(other than library)			
d. Source Code Listing			
e. Detailed Flow Charts			
8. Operating Instructions			
a. Deck Setup			
(1) Deck Sequence			
(2) Restart Sequence			
(3) Operator Instruction Card ..			

ORIGINAL PAGE IS
OF POOR QUALITY

(4) Magnetic Tape Save Labels .	_____	_____	_____
(5) Computer Time Requirements	_____	_____	_____
b. Input			
(1) Cards	_____	_____	_____
(2) Magnetic Tapes	_____	_____	_____
(3) Drum/Disc	_____	_____	_____
(4) Other	_____	_____	_____
c. Output			
(1) Cards	_____	_____	_____
(2) Magnetic Tapes	_____	_____	_____
(3) Drum/Disc	_____	_____	_____
(4) Printout	_____	_____	_____
(5) Plots	_____	_____	_____
(6) Other	_____	_____	_____
d. Restrictions and/or Limitations	_____	_____	_____
e. Diagnostics	_____	_____	_____
f. Test Case	_____	✓	_____
9. Symbols	_____	_____	_____
10. References	_____	✓	_____
11. Appendices			
a. Documentation Checklist	✓	✓	_____
b. Documentation Approval	✓	✓	_____
c. Other	_____	✓	_____

APPENDIX D
DOCUMENTATION APPROVAL

DOCUMENTATION APPROVAL

Documentation Prepared By:

Rene Sevigny
Signature

Rene Sevigny
Name (Typed)

Senior Computer Scientist
Title

6510/453-0918
Organization and Telephone No.

May 28, 1981
Date

Documentation Approved By:
(Supervisor of Person Preparing
Documentation)

Dave Johnson
Signature

Dave Johnson
Name (Typed)

Manager
Title

Project Development & Systems Support
Organization and Telephone No. Section

May 28, 1981
Date

Documentation Approved By:
Huntsville Computer Complex
(Project Officer or Monitor)

Van A. McAuley
Signature

Van McAuley
Name (Typed)

Mathematician
NASA Monitor
Title

AH33/453-2294
Organization and Telephone No.

6-5-81
May 28, 1981

Date

NASA-HSFC